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Attachment 1

Development of Elastoacoustic Integral-Equation Solver: Surface and Volumetric Integral Equations

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1 Introduction

We give below a rather complete account of the integral-equation formulations as they are being implemented in our solver for elasticity problems.

We start, in Sec. 3, with a discussion of several equivalent forms of the Lamé differential equation in elasticity, including also its first-order representation as a set of coupled equations for the displacement and the stress tensor. In addition, we derive forms of the differential equations with separated terms describing solution in the "background medium" (such as air) and interaction terms describing effects of the deviations of the medium properties from those of the background material.

Next, we discuss (in Sec. 4) the Green functions associated with the Lamé equation for the displacement field. In particular, we obtain there a form of the Green function which explicitly exhibits a nonsingular behavior of its dyadic-derivative part, which facilitates discretization of the resulting integral equations.

In the following Sections, 5 and 6, we are concerned with integral-equation formulations in elasticity, in three cases: (A) purely surface (boundary-element) equations, (B) purely volumetric (Lippmann-Schwinger, or L-S) equations, and (C) a coupled system of volume and surface equations. The last of these is a novel approach we developed, mostly in order to be able to efficiently model geometry components – in our case, the middle and inner ear – characterized by small sizes and intricate surfaces, and embedded in a larger volume of an inhomogenous material.

2 Summary of the integral equations in elasticity

We briefly the describe here the three considered types of the integral equations, and then list the genral forms of the equations themselves.

(A) Surface integral equations. The surface integral equations – or boundary integral equations, BIEs – are applicable to piecewise homogeneous materials, and provide solutions for the displacement and traction fields defined on interfaces separating different material regions. Fields in the individual regions are described in terms of the appropriate Green functions for elastic materials. We envisage using this type of equations in several situations, such as

1. Modeling of man-made objects of possibly complex geometrical shapes, but consisting of only few homogeneous materials.

2. Solution of the auxiliary surface problems arising in solution of the volumetric integral equations for materials characterized by large-contrast discontinuities in the material properties (we return to this problem below).

3. More generally, verification and checks of the solutions obtained with the volumetric-equations code in the case of piecewise homogeneous materials.

(B) Volumetric integral equations. Volumetric integral equations, on the other hand, can be used for inhomogeneous media, with (generally) different material properties assigned to the individual tetrahedra into which the volume has been discretized. We use here Lippmann-Schwinger equations with the Green function associated with the infinite (unbounded) background medium – in our case, air.

We consider two types of volumetric integral equations:

(i) Equations derived from differential equations in their first-order form. In this case the unknowns in the integral equations are the displacement and stress tensor fields defined in the considered volume.

(ii) Equations derived from differential equations in their second-order form. In this formulation the unknowns are only the components of the displacement field.

In both cases we discretize the integral equations in terms of piecewise linear basis functions. Each such basis function is associated with the vertices of the tetrahedral mesh, and supported on sets of tetrahedra adjacent to the considered vertex.

In designing our integral-equation formulation we pay a particular attention to the problem of a possible discontinuous behavior of the material properties, which is, clearly, always present when considering a mechanically dense (biological) material immersed in air.

Such problems are known to cause difficulties in solving integral equations in acoustics and, in that case, we have devised an approach [1] in which the original system of equations is reformulated in terms of a surface problem associated with the contrast interface(s) (characterized by a large ratio of densities of the adjacent materials) and a "residual" volumetric problem. The analogous problem in elasticity appears to be considerably more complex, and we have put much effort into deriving appropriate forms of integral equations, in both first- and second-order formulations ((i) and (ii) above).

(C) Coupled volume-surface integral equations. A coupled system of volumetric and surface integral equations arises, e.g., when a homogeneous material region is embedded, as an inclusion, in an inhomogeneous material. We briefly summarize the structure of such a system of equations below.

General forms of the integral equations. We give below formulae for the systems of integral equations used in this Report. The derivations are given and properties of these equations are discussed in detail in Sections 5 and 6.

(A) Surface integral equations. We first present the general form of the surface integral equations for a set of homogenous regions Ω_m separated by interfaces; one of these regions, Ω_0, is the unbounded background medium. The displacement and traction fields are assumed to be continuous across the interfaces.

The resulting system of integral equations simply consists of two equations per interface (oriented surface) S_{mn} separating the regions Ω_m (on the negative side of the interface) and

Ω_n (on its positive side),

$$\frac{1}{2}\,\mathbf{u}(\mathbf{r}) + \int_{S_{mn}} \mathrm{d}^2 r' \left[\Gamma_m^{\mathrm{T}}(\mathbf{t},\mathbf{r}')\cdot\mathbf{u}(\mathbf{r}') + G_m^{\mathrm{T}}(\mathbf{r},\mathbf{r}')\cdot\mathbf{t}(\mathbf{r}')\right]$$
$$- \sum_{\substack{S_{im}\in\partial\Omega_m \\ i\neq n}} \int_{S_{im}} \mathrm{d}^2 r' \left[\Gamma_m^{\mathrm{T}}(\mathbf{t},\mathbf{r}')\cdot\mathbf{u}(\mathbf{r}') + G_m^{\mathrm{T}}(\mathbf{r},\mathbf{r}')\cdot\mathbf{t}(\mathbf{r}')\right] = \delta_{m0}\,\mathbf{u}^{\mathrm{in}}(\mathbf{r}) \text{ for } \mathbf{r}\in S_{mn}\ , \quad (2.1\mathrm{a})$$

$$\frac{1}{2}\,\mathbf{u}(\mathbf{r}) - \int_{S_{mn}} \mathrm{d}^2 r' \left[\Gamma_n^{\mathrm{T}}(\mathbf{t},\mathbf{r}')\cdot\mathbf{u}(\mathbf{r}') + G_n^{\mathrm{T}}(\mathbf{r},\mathbf{r}')\cdot\mathbf{t}(\mathbf{r}')\right]$$
$$+ \sum_{\substack{S_{nj}\in\partial\Omega_n \\ j\neq m}} \int_{S_{nj}} \mathrm{d}^2 r' \left[\Gamma_n^{\mathrm{T}}(\mathbf{t},\mathbf{r}')\cdot\mathbf{u}(\mathbf{r}') + G_n^{\mathrm{T}}(\mathbf{r},\mathbf{r}')\cdot\mathbf{t}(\mathbf{r}')\right] = \delta_{n0}\,\mathbf{u}^{\mathrm{in}}(\mathbf{r}) \quad \text{for } \mathbf{r}\in S_{mn}\ . \quad (2.1\mathrm{b})$$

With reference to Fig. 1, Eq.(2.1a) represents contributions to the displacement field $\mathbf{u}$ on the interface S_{mn} due to the displacement and traction fields $\mathbf{u}$ and $\mathbf{t}$ on the same interface (the first integral) and on other interfaces, S_{im}, forming boundaries of the region Ω_m with other regions Ω_i, $i \neq n$. These intervals involve Green functions G_m and Γ_m (defined by Eqs. (4.20) and (5.4) in Sec. 5.1), describing propagation of the fields in the region Ω_m. Similarly, Eq.(2.1b) represents contributions to the field $\mathbf{u}$ on the interface S_{mn} due to the fields on the boundaries of the other region, Ω_n, adjacent to the interface. The r.h.s.s of Eqs. (2.1) are the incident fields due to distant sources in the region Ω_0 (hence the delta-functions δ_{m0} and δ_{n0}).

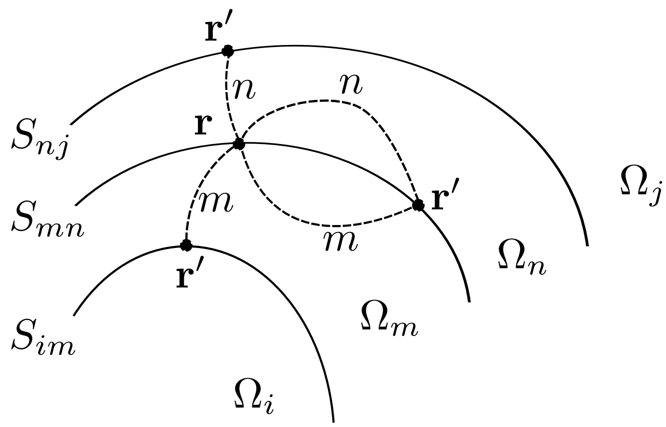

Figure 1: A schematic representation of regions Ω and interfaces S appearing in integral equations 2.1.

(B) Volumetric integral equations. We obtained our volumetric equations are the Lippmann-Schwinger (L-S) equations, describing the elastic fields as propagating in the background medium (characterized by some density ρ_0 and Lamé coefficients λ_0 and μ_0), modified by the presence of the actual medium with material parameters ρ, λ, and μ. The interaction of the elastic wave with the medium may be described in many equivalent ways,

resulting in various forms of the L-S equation. Our forms of these equations are not the conventionally used ones, as we took special care to ensure their favorable properties in problems involving large density contrasts.

(B i) Equations in the "first-order" form. In this formulation, derived from the Lamé equation in its first-order form, the unknowns are the velocity $v_i := -\mathrm{i}\, k\, u_i$ (where k is the wave number in the background medium), the pressure $p := -\frac{1}{3}\,\tau_{kk}$, and the symmetric traceless part σ_{ij} of the stress tensor τ_{ij}. The equations involve the Green function $g(r) = \exp(\mathrm{i}kr)/(4\pi r)$ of the Helmholtz equation in the background medium, as well as its derivatives,

$$g_{mn}(\mathbf{r}) := \left(\tfrac{1}{3}\,\delta_{mn}\,k^2 + \partial_m\partial_n\right) g(\mathbf{r}) \ . \tag{2.2}$$

The obtained system of integral equations, Eqs. (6.35), is then

$$\begin{aligned}
\frac{\rho(\mathbf{r})}{\rho_0}\,v_i(\mathbf{r}) &+ \int \mathrm{d}^3r'\,\left(\partial_i\partial_m\,g(\mathbf{r}-\mathbf{r}')\right)\left(\frac{\rho(\mathbf{r}')}{\rho_0}-1\right)v_m(\mathbf{r}') \\
&+ \frac{1}{k^2}\,\partial_m\left[\frac{\mu(\mathbf{r})}{\lambda_0}\left(\partial_i\,v_m(\mathbf{r}) + \partial_m\,v_i(\mathbf{r})\right)\right] \\
&+ \frac{1}{k^2}\int \mathrm{d}^3r'\,\left(\partial_i\,g_{mn}(\mathbf{r}-\mathbf{r}')\right)\frac{2\mu(\mathbf{r}')}{\lambda_0}\,\partial'_m\,v_n(\mathbf{r}') \\
&+ \frac{\mathrm{i}\,k}{\lambda_0}\int \mathrm{d}^3r'\,\left(\partial_i\,g(\mathbf{r}-\mathbf{r}')\right)\left(\varphi(\mathbf{r}')-1\right)p(\mathbf{r}') \\
&= v_i^{\mathrm{in}}(\mathbf{r}) \ , \\
p(\mathbf{r}) - k^2 &\int \mathrm{d}^3r'\,g(\mathbf{r}-\mathbf{r}')\left(\varphi(\mathbf{r}')-1\right)p(\mathbf{r}') \\
&+ \frac{2\mathrm{i}}{3k}\,\frac{\mu(\mathbf{r})}{\lambda_0}\,\partial_m\,v_m(\mathbf{r}) + \frac{\mathrm{i}}{k}\int \mathrm{d}^3r'\,g_{mn}(\mathbf{r}-\mathbf{r}')\,\frac{2\mu(\mathbf{r}')}{\lambda_0}\,\partial'_m\,v_n(\mathbf{r}') \\
&= p^{\mathrm{in}}(\mathbf{r}) \ , \\
\sigma_{ij}(\mathbf{r}) &- \frac{\mathrm{i}}{k}\,\frac{\mu(\mathbf{r})}{\lambda_0}\left[\partial_i\,v_j(\mathbf{r}) + \partial_j\,v_i(\mathbf{r}) - \tfrac{2}{3}\,\delta_{ij}\,\partial_m\,v_m(\mathbf{r})\right] \\
&= \sigma_{ij}^{\mathrm{in}}(\mathbf{r}) \ ,
\end{aligned} \tag{2.3}$$

with a dimensionless material parameter

$$\varphi = \frac{\lambda_0}{\lambda + \frac{2}{3}\mu} \ . \tag{2.4}$$

(B ii) Equation in the "second-order" form. In this case we have only a single equation Eq.(6.51) for the three-component displacement field $\mathbf{u}$,

$$
\begin{aligned}
u_i(\mathbf{r}) - k^{-2}\,\partial_j\, & \Big[\big(1-\xi_\lambda(\mathbf{r})\big)\,\delta_{ij}\partial_k u_k(\mathbf{r}) - \xi_\mu(\mathbf{r})\,\Big(\partial_i u_j(\mathbf{r}) + \partial_j u_i(\mathbf{r})\Big)\Big] \\
& - k^{-2}\left(\partial_j \frac{\rho_0}{\rho(\mathbf{r})}\right) \\
& \qquad \Big[\eta_\lambda(\mathbf{r})\;\delta_{ij}\,\partial_k u_k(\mathbf{r}) + \eta_\mu(\mathbf{r})\,\Big(\partial_i u_j(\mathbf{r}) + \partial_j u_i(\mathbf{r})\Big)\Big] \\
& - k^{-2}\int \mathrm{d}^3 r'\,\partial_i\,\partial_l\,\partial_j\, g(\mathbf{r}-\mathbf{r}') \\
& \qquad \Big[\big(1-\xi_\lambda(\mathbf{r}')\big)\,\delta_{lj}\,\partial'_k u_k(\mathbf{r}') - \xi_\mu(\mathbf{r}')\,\Big(\partial'_l u_j(\mathbf{r}') + \partial'_j u_l(\mathbf{r}')\Big)\Big] \\
& - k^{-2}\int \mathrm{d}^3 r'\,\partial_i\,\partial_l\, g(\mathbf{r}-\mathbf{r}')\left(\partial'_j\,\frac{\rho_0}{\rho(\mathbf{r}')}\right) \\
& \qquad \Big[\eta_\lambda(\mathbf{r}')\;\delta_{lj}\,\partial'_k u_k(\mathbf{r}') + \eta_\mu(\mathbf{r}')\,\Big(\partial'_l u_j(\mathbf{r}') + \partial'_j u_l(\mathbf{r}')\Big)\Big] \\
& = u_i^{\mathrm{in}}(\mathbf{r})\ ,
\end{aligned}
\tag{2.5}
$$

with the auxiliary material-dependent coefficients defined as

$$
\xi_\lambda = \frac{\rho_0}{\rho}\,\frac{\lambda}{\lambda_0}\ , \quad \xi_\mu = \frac{\rho_0}{\rho}\,\frac{\mu}{\lambda_0}\ , \quad \eta_\lambda = \frac{\lambda}{\lambda_0}\ , \quad \eta_\mu = \frac{\mu}{\lambda_0}\ . \tag{2.6}
$$

Properties of the integral equations in high-contrast problems. The volumetric integral equations (2.3) and (2.5) have quite different (although equivalent) forms; they share, however, common features, which become relevant in problems involving large contrast. Such cases, in our applications, are characterized by large ratios of material density and the Lamé parameter λ values in the considered material and in the background medium, with moderate values of the wave propagation speed, i.e.,

$$
\frac{\rho}{\rho_0} \sim \frac{\lambda}{\lambda_0} \gg 1\ . \tag{2.7}
$$

In this limit only some terms in the integral equations are dominant and, moreover, they represent contributions of interfaces at which there occur large jumps in the parameters ρ and λ. This structure of the equations facilitates their discretization and solution in high-contrast problems.

(C) Coupled volumetric and surface integral equations. A simple example of a system involving both volumetric and surface fields is visualized in Fig. 2. In this case surface fields $\mathbf{u}$ and $\mathbf{t}$ are defined on the boundary $\partial\Omega_m$ of a homogeneous region Ω_m embedded in an inhomogeneous region Ω, supporting the volumetric field $\mathbf{u}$.

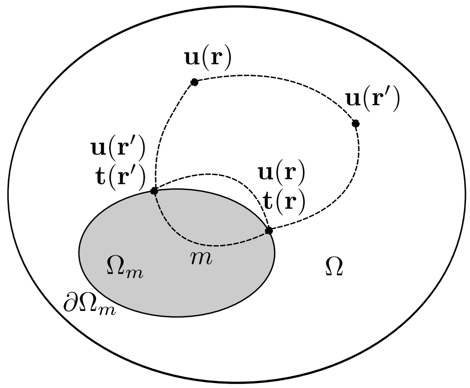

Figure 2: A schematic representation of coupled integral equations: a volume integral equation for the displacement field $\mathbf{u}$ in the inhomogeneous region Ω and a surface integral equation for the displacement and traction fields, $\mathbf{u}$ and $\mathbf{t}$, on the boundary of the homogeneous material region Ω_m embedded in Ω.

In notation similar to that in Eqs. (2.1), the resulting coupled integral equations have then the general form

$$
\begin{aligned}
\mathbf{u}(\mathbf{r}) &- \int_\Omega \mathrm{d}^3 r'\, G(\mathbf{r}-\mathbf{r}')\, \mathcal{S}(\mathbf{u}(\mathbf{r}')) \\
&- \int_{\partial\Omega_m} \mathrm{d}^2 r' \left[\Gamma^{\mathrm{T}}(\mathbf{t},\mathbf{r}') \cdot \mathbf{u}(\mathbf{r}') + G^{\mathrm{T}}(\mathbf{r},\mathbf{r}') \cdot \mathbf{t}(\mathbf{r}')\right] \\
&= \mathbf{u}^{\mathrm{in}}(\mathbf{r}) \qquad\qquad \text{for } \mathbf{r} \in \Omega \;, \qquad (2.8\mathrm{a}) \\
\tfrac{1}{2}\,\mathbf{u}(\mathbf{r}) &- \int_{\partial\Omega_m} \mathrm{d}^2 r' \left[\Gamma_m^{\mathrm{T}}(\mathbf{t},\mathbf{r}') \cdot \mathbf{u}(\mathbf{r}') + G_m^{\mathrm{T}}(\mathbf{r},\mathbf{r}') \cdot \mathbf{t}(\mathbf{r}')\right] \\
&= 0 \qquad\qquad \text{for } \mathbf{r} \in \partial\Omega_m \;, \qquad (2.8\mathrm{b}) \\
\tfrac{1}{2}\,\mathbf{u}(\mathbf{r}) &+ \int_{\partial\Omega_m} \mathrm{d}^2 r' \left[\Gamma^{\mathrm{T}}(\mathbf{t},\mathbf{r}') \cdot \mathbf{u}(\mathbf{r}') + G^{\mathrm{T}}(\mathbf{r},\mathbf{r}') \cdot \mathbf{t}(\mathbf{r}')\right] \\
&- \int_\Omega \mathrm{d}^3 r'\, G(\mathbf{r}-\mathbf{r}')\, \mathcal{S}(\mathbf{u}(\mathbf{r}')) \\
&= \mathbf{u}^{\mathrm{in}}(\mathbf{r}) \qquad\qquad \text{for } \mathbf{r} \in \partial\Omega_m \;, \qquad (2.8\mathrm{c})
\end{aligned}
$$

where $\mathcal{S}(\mathbf{u}(\mathbf{r}))$ is a functional of the displacement field, representing a volumetric source, whose specific form depends on the implementation of the volumetric (Lippmann-Schwinger) equations. The Green functions labeled with the index m refer to the material of the region Ω_m, while those without the label are the background-medium Green functions.

3 Differential equations in elasticity

3.1 Second-order differential equations for isotropic media

General Lamé equation. From the frequency-domain elasticity equation for the displacement field $\mathbf{u}(\mathbf{r})$,

$$\omega^2 \rho u_i + \partial_j \tau_{ij} = 0 , \tag{3.1}$$

the constitutive relation

$$\tau_{ij} = C_{ijkl} \epsilon_{kl} , \tag{3.2}$$

and the definition of the strain tensor,

$$\epsilon_{ij} = \tfrac{1}{2} (\partial_i u_j + \partial_j u_i) , \tag{3.3}$$

one obtains, upon setting

$$C_{ijkl} = \lambda \delta_{ij} \delta_{kl} + \mu (\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}) , \tag{3.4}$$

the basic form of the Lamé equation

$$\omega^2 \rho u_i + \partial_i (\lambda \partial_j u_j) + \partial_j \left[\mu \left(\partial_i u_j + \partial_j u_i\right)\right] = 0 . \tag{3.5}$$

The above equation is equivalent to the set of two first order equations, Eq.(3.1) and the definition of the stress tensor in terms of the displacement,

$$\tau_{ij} = \lambda \delta_{ij} \partial k u_k + \mu \left(\partial_i u_j + \partial_j u_i\right) . \tag{3.6}$$

In order to derive the L-S equation for elasticity, we now represent Eq.(3.5) in a form exhibiting the background-medium operator and interaction terms. The background material is characterized by the density ρ_0 and the Lamé coefficients λ_0 and $\mu_0 \equiv 0$, such that the wave vector k in that medium is

$$k^2 = \frac{\rho_0}{\lambda_0} \omega^2 . \tag{3.7}$$

In terms of k, the basic form of the Lamé equation (3.5) is

$$k^2 \frac{\rho}{\rho_0} u_i + \partial_i \left(\frac{\lambda}{\lambda_0} \partial_j u_j\right) + \partial_j \left[\frac{\mu}{\lambda_0} \left(\partial_i u_j + \partial_j u_i\right)\right] = 0 . \tag{3.8}$$

Lamé equation in L-S form. We will use ***three*** alternative forms of the differential equation, equivalent to Eq.(3.8),

$$\left(\partial_i\partial_j + \delta_{ij}\,k^2\right)\,u_j - k^2\left(1-\frac{\rho}{\rho_0}\right)u_i - \partial_i\left[\left(1-\frac{\lambda}{\lambda_0}\right)\partial_j u_j\right] + \partial_j\left[\frac{\mu}{\lambda_0}\,\left(\partial_i u_j + \partial_j u_i\right)\right] = 0\ , \tag{3.9a}$$

$$\left(\partial_i\partial_j + \delta_{ij}\,k^2\right)\,u_j - \partial_i\left[\left(1-\frac{\rho_0\,\lambda}{\rho\,\lambda_0}\right)\partial_j u_j\right] + \frac{\rho_0}{\rho}\,\partial_j\left[\frac{\mu}{\lambda_0}\,\left(\partial_i u_j + \partial_j u_i\right)\right] - \left(\partial_i\frac{\rho_0}{\rho}\right)\frac{\lambda}{\lambda_0}\,\partial_j u_j = 0\ , \tag{3.9b}$$

$$\left(\partial_i\partial_j + \delta_{ij}\,k^2\right)\,u_j - \partial_j\left[\left(1-\xi_\lambda\right)\delta_{ij}\,\partial_l u_l - \xi_\mu\left(\partial_i u_j + \partial_j u_i\right)\right] - \left(\partial_j\frac{\rho_0}{\rho}\right)\left[\eta_\lambda\,\delta_{ij}\,\partial_l u_l + \eta_\mu\,\left(\partial_i u_j + \partial_j u_i\right)\right] = 0\ , \tag{3.9c}$$

where the dimensionless parameters ξ_λ, ξ_μ, η_λ, and η_μ are defined as

$$\xi_\lambda = \frac{\rho_0}{\rho}\,\frac{\lambda}{\lambda_0}\ , \qquad \xi_\mu = \frac{\rho_0}{\rho}\,\frac{\mu}{\lambda_0}\ . \tag{3.10}$$

and

$$\eta_\lambda = \frac{\lambda}{\lambda_0}\ , \qquad \eta_\mu = \frac{\mu}{\lambda_0}\ . \tag{3.11}$$

In air we have, by definition, $\xi_\lambda = \eta_\lambda = 1$ and $\xi_\mu = \eta_\mu = 0$, while in typical biological media $\rho_0/\rho \ll 1$, $\eta_\lambda \gg 1$, and $\eta_\mu \gg 1$, but the coefficients ξ_λ and ξ_μ (which are proportional to the refraction coefficients squared) remain of order 1.

The heuristics behind Eq.(3.9b) involves representing the pressure in terms of the displacement, $p = -\lambda\,\partial_i u_i$, "removing" one differentiation, and adding the shear term with the Lamé coefficient μ. An important feature of Eq.(3.9b) is the last term with the manifestly appearing gradient of ρ_0/ρ.

Similar remarks apply to Eq.(3.9c), in which, additionally, the terms proportional to ξ_λ and ξ_μ combine to form expressions proportional to the stress tensor (see Eq.(6.52) below).

3.2 Second-order differential equations for anisotropic media

In the following we will also consider equations for anisotropic media; the main reason for this is that we will impose kinematic constraints in elastic shell theories by means of anisotropic material properties. In addition, we may need to model anisotropic shells, such as the basilar membrane.

For an anisotropic medium the elasticity tensor C of Eq.(3.2) is a general fourth rank tensor satisfying the symmetry relations

$$C_{ijkl} = C_{jikl}\ , \quad C_{ijkl} = C_{ijlk}\ , \quad C_{ijkl} = C_{klij}\ , \tag{3.12}$$

and the condition that the quadratic form

$$W := C_{ijkl}\,\epsilon_{ij}\,\epsilon_{kl} \tag{3.13}$$

is positive-definite. The symmetry properties (3.12) imply that the tensor C involves 21 independent material parameters.

With a general elasticity tensor C, the frequency-domain form of Eq.(3.1) becomes, in analogy to Eq.(3.8),

$$k^2 \frac{\rho}{\rho_0} u_i + \frac{1}{2\lambda_0} \partial_j \left[C_{ijkl} \left(\partial_k u_l + \partial_l u_k\right)\right] = 0 \; . \tag{3.14}$$

3.3 First-order differential equations for isotropic media

General first-order equations. The second-order Lamé equation (3.8) can be then written as a system of two first-order equations

$$k^2 \frac{\rho}{\rho_0} u_i + \frac{1}{\lambda_0} \partial_j \tau_{ij} = 0 \; , \tag{3.15a}$$

$$\tau_{ij} - \lambda \, \delta_{ij} \, \partial_k u_k - \mu \left(\partial_i u_j + \partial_j u_i\right) = 0 \; , \tag{3.15b}$$

containing no derivatives of material parameters.

As a matter of notation, we define the "velocity" $\mathbf{v}$ as

$$\mathbf{v} = -\,\mathrm{i}\, k \, \mathbf{u} \tag{3.16}$$

and rewrite the above equations in the form

$$\mathrm{i}\, k \frac{\rho}{\rho_0} v_i + \frac{1}{\lambda_0} \partial_j \tau_{ij} = 0 \; , \tag{3.17a}$$

$$\mathrm{i}\, k \, \tau_{ij} + \lambda \, \delta_{ij} \, \partial_k v_k + \mu \left(\partial_i v_j + \partial_j v_i\right) = 0 \; . \tag{3.17b}$$

Next, we try to represent these equations in such a form that the material parameters do not appear as factors of the differential operators. At the same time, it should be possible to split those equations into terms describing fields in the background medium ($\rho = \rho_0$, $\lambda = \lambda_0$, $\mu = 0$) and interaction terms; this structure is required in order to derive the L-S equations.

A straightforward decomposition into background and interaction terms. We represent now Eqs. (3.17) as

$$\mathrm{i}\, k \, v_i + \frac{1}{\lambda_0} \partial_j \tau_{ij} + \mathrm{i}\, k \left(\frac{\rho}{\rho_0} - 1\right) v_i = 0 \; , \tag{3.18a}$$

$$\mathrm{i}\, k \frac{1}{\lambda_0} \sigma_{ij} + \delta_{ij} \, \partial_k v_k + \delta_{ij} \left(\frac{\lambda}{\lambda_0} - 1\right) \partial_k v_k + \frac{\mu}{\lambda_0} \left(\partial_i v_j + \partial_j v_i\right) = 0 \tag{3.18b}$$

or

$$\mathcal{K} \, \mathcal{F} \equiv \left(\mathcal{D} + \mathcal{V}\right) \mathcal{F} = 0 \tag{3.19}$$

with

$$\left[\begin{array}{c:c} \mathcal{D}^{\mathrm{vv}}_{ik} & \mathcal{D}^{\mathrm{v}\omega}_{ikl} \\ \hdashline \mathcal{D}^{\omega\mathrm{v}}_{ijk} & \mathcal{D}^{\omega\omega}_{ijkl} \end{array}\right] = \left[\begin{array}{c:c} \mathrm{i}\, k \, \delta_{ik} & \delta_{ik} \, \partial_l \\ \hdashline \delta_{ij} \, \partial_k & \mathrm{i}\, k \, \delta_{ik} \, \delta_{jl} \end{array}\right] \; , \tag{3.20}$$

$$\left[\begin{array}{c:c} \mathcal{V}^{\mathrm{vv}}_{ik} & \mathcal{V}^{\mathrm{v}\omega}_{ikl} \\ \hdashline \mathcal{V}^{\omega\mathrm{v}}_{ijk} & \mathcal{V}^{\omega\omega}_{ijkl} \end{array}\right] = \left[\begin{array}{c:c} \mathrm{i}\,k\,\delta_{ik}\,(\lambda/\lambda_0 - 1) & 0 \\ \hdashline \delta_{ij}\,(\lambda/\lambda_0 - 1)\,\partial_k + \mu/\lambda_0\,(\delta_{ik}\,\partial_j + \delta_{jk}\,\partial_i) & 0 \end{array}\right] , \tag{3.21}$$

and

$$\left[\begin{array}{c} \mathcal{F}^{\mathrm{v}}_i \\ \hdashline \mathcal{F}^{\omega}_{ij} \end{array}\right] = \left[\begin{array}{c} v_i \\ \hdashline \omega_{ij} \end{array}\right] \equiv \left[\begin{array}{c} v_i \\ \hdashline \sigma_{ij}/\lambda_0 \end{array}\right] \tag{3.22}$$

The Green function corresponding to the background-medium differential operator (3.20) is defined by the equation

$$\mathcal{D}\,\mathcal{G}(\mathbf{r}) = -\,\mathcal{I}\,\delta^2(\mathbf{r}) , \tag{3.23}$$

where $\mathcal{I}$ is the unit tensor (we discuss more general Green functions for elastic media in Sec. 4).

By taking the Fourier transform of Eq.(3.23) we can obtain an algebraic equation for the Fourier representation

$$\mathcal{G}(\mathbf{r}) = \int \frac{\mathrm{d}^3 q}{(2\pi)^3}\,\mathrm{e}^{\mathrm{i}\,\mathbf{q}\cdot\mathbf{r}}\,\widetilde{\mathcal{G}}(\mathbf{q}) \tag{3.24}$$

of the Green function. It has the form

$$\left[\begin{array}{c:c} \mathrm{i}\,k\,\delta_{ik} & -\,\mathrm{i}\,\delta_{ik}\,q_l \\ \hdashline -\,\mathrm{i}\,\delta_{ij}\,q_k & \mathrm{i}\,k\,\delta_{ik}\,\delta_{jl} \end{array}\right] \left[\begin{array}{c:c} \widetilde{\mathcal{G}}^{\mathrm{vv}}_{km} & \widetilde{\mathcal{G}}^{\mathrm{v}\omega}_{kmn} \\ \hdashline \widetilde{\mathcal{G}}^{\omega\mathrm{v}}_{klm} & \widetilde{\mathcal{G}}^{\omega\omega}_{klmn} \end{array}\right] (\mathbf{q}) = -\left[\begin{array}{c:c} \delta_{im} & 0 \\ \hdashline 0 & \frac{1}{2}\,(\delta_{im}\,\delta_{jn} + \delta_{in}\,\delta_{jm}) \end{array}\right] . \tag{3.25}$$

Separation of dilatational and distortional components. In order to disentangle the dependences of equations on the Lamé coefficients λ and μ, we separate the stress tensors into its volumetric (dilatational) part, related to the pressure, and distortional (deviatoric) part, related to shear deformations. We decompose the stress tensor τ as

$$\tau_{ij} = -\,\delta_{ij}\,p + \sigma_{ij} , \tag{3.26}$$

where

$$p := -\,\tfrac{1}{3}\,\mathrm{tr}\,\tau \equiv -\tfrac{1}{3}\,\tau_{kk} \tag{3.27}$$

is the pressure. The tensor σ is then, by construction, symmetric and traceless.

By substituting the decomposition (3.26) in Eqs. (3.17) we find

$$\mathrm{i}\,k\,\frac{\rho}{\rho_0}\,v_i - \frac{1}{\lambda_0}\,\partial_i\,p + \frac{1}{\lambda_0}\,\partial_j\,\sigma_{ij} = 0 , \tag{3.28a}$$

$$\mathrm{i}\,k\,p - (\lambda + \tfrac{2}{3}\mu)\,\partial_k\,v_k = 0 , \tag{3.28b}$$

$$\mathrm{i}\,k\,\sigma_{ij} + \mu\,(\partial_i\,v_j + \partial_j\,v_i - \tfrac{2}{3}\,\delta_{ij}\,\partial_k\,v_k) = 0 ; \tag{3.28c}$$

Eq.(3.28b) is obtained by taking the trace of Eq.(3.17b). The desired form of the differential equations is then simply

$$\mathrm{i}\,k\,\frac{\rho}{\rho_0}\,v_i - \frac{1}{\lambda_0}\,\partial_i\,p + \frac{1}{\lambda_0}\,\partial_j\,\sigma_{ij} = 0 , \tag{3.29a}$$

$$\mathrm{i}\,k\,\varphi\,p - \lambda_0\,\partial_k\,v_k = 0 , \tag{3.29b}$$

$$\mathrm{i}\,k\,\sigma_{ij} + \mu\,(\partial_i\,v_j + \partial_j\,v_i - \tfrac{2}{3}\,\delta_{ij}\,\partial_k\,v_k) = 0 , \tag{3.29c}$$

with a dimensionless parameter

$$\varphi = \frac{\lambda_0}{\lambda + \frac{2}{3}\mu} \ . \tag{3.30}$$

We did not eliminate the Lamé coefficient μ multiplying the derivatives in Eq.(3.29c); had we divided that equation by μ, the background medium limit $\mu \to 0$ would not exist.

Equations in the L-S form. In the following we will represent Eqs. (3.29) in the matrix operator form as

$$\mathcal{K}\,\mathcal{F} = 0 \ , \tag{3.31}$$

where the solution (field) vector $\mathcal{F}$ is defined as

$$\mathcal{F} = \left[v_i \,\vdots\, p \,\vdots\, \sigma_{ij} \right]^{\mathrm{T}} \tag{3.32}$$

and the action of the operator $\mathcal{K}$, say, $\mathcal{F}' = \mathcal{K}\,\mathcal{F}$, is represented as

$$\begin{bmatrix} v'_i \\ p' \\ \sigma'_{ij} \end{bmatrix} = \begin{bmatrix} \mathcal{K}^{\mathrm{vv}}_{ik} & \mathcal{K}^{\mathrm{vp}}_{i} & \mathcal{K}^{\mathrm{v}\sigma}_{ikl} \\ \mathcal{K}^{\mathrm{pv}}_{k} & \mathcal{K}^{\mathrm{pp}} & \mathcal{K}^{\mathrm{p}\sigma}_{kl} \\ \mathcal{K}^{\sigma\mathrm{v}}_{ijk} & \mathcal{K}^{\sigma\mathrm{p}}_{ij} & \mathcal{K}^{\sigma\sigma}_{ijkl} \end{bmatrix} \begin{bmatrix} v_k \\ p \\ \sigma_{kl} \end{bmatrix} . \tag{3.33}$$

The above equation illustrates our indexing conventions: elements of a set of functions (v, p, σ) are assigned three possible sets of indices: $(i, \ , ij)$ or $(k, \ , kl)$ or $(m, \ , mn)$.

In order to derive the L-S equations, we split the operator $\mathcal{K}$ as $\mathcal{K} = \mathcal{D} + \mathcal{V}$, where $\mathcal{D}$ describes the fields in the background medium, and $\mathcal{V}$ the remaining interactions. We then define the Green function $\mathcal{G}$ as the negative of the inverse of the operator $\mathcal{D}$, or, more physically, as a field generated by a point-like "unit" source, i.e., a solution of the equation

$$\mathcal{D}\,\mathcal{G}(\mathbf{r}) = -\,\mathcal{I}\,\delta^2(\mathbf{r}) \ , \tag{3.34}$$

where $\mathcal{I}$ is an appropriately defined "unit" tensor. In our case we have to keep in mind that the symmetric traceless tensor field σ has to be generated by a source satisfying those constraints; hence the tensor $\mathcal{I}$ must be symmetric and traceless in the indices associated with the field σ.

In our case the system of equations (3.34) for the Green function takes the form

$$\begin{aligned} &\begin{bmatrix} \mathrm{i}\,k\,\delta_{ik} & -\,\partial_i & \delta_{ik}\,\partial_l \\ -\,\partial_k & \mathrm{i}\,k & 0 \\ 0 & 0 & \mathrm{i}\,k\,\delta_{ik}\,\delta_{jl} \end{bmatrix} \begin{bmatrix} \mathcal{G}^{\mathrm{vv}}_{km} & \mathcal{G}^{\mathrm{vp}}_{k} & \mathcal{G}^{\mathrm{v}\sigma}_{kmn} \\ \mathcal{G}^{\mathrm{pv}}_{m} & \mathcal{G}^{\mathrm{pp}} & \mathcal{G}^{\mathrm{p}\sigma}_{mn} \\ \mathcal{G}^{\sigma\mathrm{v}}_{klm} & \mathcal{G}^{\sigma\mathrm{p}}_{kl} & \mathcal{G}^{\sigma\sigma}_{klmn} \end{bmatrix} (\mathbf{r}) \\ &\qquad = -\begin{bmatrix} \delta_{im} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \Delta_{ijmn} \end{bmatrix} \delta^3(\mathbf{r}) \ , \end{aligned} \tag{3.35}$$

where the tensor

$$\Delta_{ijmn} := \tfrac{1}{2}\left(\delta_{im}\,\delta_{jn} + \delta_{in}\,\delta_{jm} - \tfrac{2}{3}\,\delta_{ij}\,\delta_{mn}\right) \tag{3.36}$$

defines a symmetric and traceless source of the field σ. It is also an idempotent (or projection) operator,

$$\Delta_{ijkl}\,\Delta_{klmn} = \Delta_{ijmn}\ , \tag{3.37}$$

which follows immediately from the tracelessness property,

$$\Delta_{iikl} = 0 = \Delta_{ijkk}\ , \tag{3.38}$$

and implies

$$\mathcal{I}^2 = \mathcal{I}. \tag{3.39}$$

Having specified the background medium operator $\mathcal{D}$ (Eq.(3.35)), we define the interaction term as $\mathcal{V} := \mathcal{K} - \mathcal{D}$. From the system of equations (3.29), with Eq.(3.29c) written as

$$\mathrm{i}\,k\,\sigma_{ij} + 2\mu\,\Delta_{ijlk}\,\partial_l\,v_k = 0\ , \tag{3.40}$$

we find

$$\mathcal{V} = \left[\begin{array}{c:c:c} \mathcal{V}^{\mathrm{vv}}_{ik} & \mathcal{V}^{\mathrm{vp}}_{i} & \mathcal{V}^{\mathrm{v}\sigma}_{ikl} \\ \hdashline \mathcal{V}^{\mathrm{pv}}_{k} & \mathcal{V}^{\mathrm{pp}} & \mathcal{V}^{\mathrm{p}\sigma}_{kl} \\ \hdashline \mathcal{V}^{\sigma\mathrm{v}}_{ijk} & \mathcal{V}^{\sigma\mathrm{p}}_{ij} & \mathcal{V}^{\sigma\sigma}_{ijkl} \end{array}\right] = \left[\begin{array}{c:c:c} \mathrm{i}\,k\,(\rho-1)\,\delta_{ik} & 0 & 0 \\ \hdashline 0 & \mathrm{i}\,k\,(\varphi-1) & 0 \\ \hdashline 2\mu\,\Delta_{ijlk}\,\partial_l & 0 & 0 \end{array}\right]\ . \tag{3.41}$$

In order to simplify the notation, we have temporarily set $\rho_0 = \lambda_0 = 1$; these parameters will be restored in the final form of the integral equations.

We note that the coupling between the "acoustic fields" ($\mathbf{v}$ and p) and the "shear field" σ is given here by a differential operator proportional to μ. It is also important to note that the Green function $\mathcal{G}$ and the operator (3.41) satisfy, by construction, the projection conditions

$$\mathcal{G}\,\mathcal{I} = \mathcal{G} = \mathcal{I}\,\mathcal{G} \tag{3.42}$$

and

$$\mathcal{V}\,\mathcal{I} = \mathcal{V} = \mathcal{I}\,\mathcal{V}\ . \tag{3.43}$$

3.4 An alternative form of differential equations (for isotropic media) in the L-S form

We derive here yet another form of differential equations, which may be well suited as a basis of the L-S equation for high contrast problems. As a guideline we will use the behavior of various physical quantities at material interfaces at which the density (and other parameters) are discontinuous: some of the quantities are continuous across such interfaces, and some not.

We start with the Lamé equation in the first-order, Eq.(3.8), and temporarily set $\rho_0 = \lambda_0 = 1$,

$$k^2\,\rho\,u_i + \partial_j\,\tau_{ij} = 0\ , \tag{3.44a}$$

$$\tau_{ij} - \lambda\,\delta_{ij}\,\partial_k\,u_k - \mu\left(\partial_i\,u_j + \partial_j\,u_i\right) = 0\ . \tag{3.44b}$$

On this basis, we will first obtain, in a very elementary way, two complementary equations, one for the pressure and other for the displacement, in both of which the discontinuity of material parameters is "isolated" in a similar way. We will then try to generalize those equations to the case of elasticity.

Acoustics. For acoustics ($\mu = 0$), Eqs. (3.44) become

$$k^2\,\rho\,u_i + \partial_j\,\tau_{ij} = 0\ , \tag{3.45a}$$

$$\tau_{ij} - \lambda\,\delta_{ij}\,\partial_l\,u_l = 0\ . \tag{3.45b}$$

By representing the stress tensor in terms of the pressure p,

$$\tau_{ij} = -\,\delta_{ij}\,p\ , \tag{3.46}$$

one obtains a system of coupled first-order equations

$$k^2\,\rho\,u_i - \partial_i\,p = 0\ , \tag{3.47a}$$

$$p + \lambda\,\partial_l\,u_l = 0\ . \tag{3.47b}$$

Acoustics: L-S form of equations for the pressure. After dividing Eq.(3.47a) by ρ, taking its divergence, and eliminating the displacement, we obtain the usual second-order equation for pressure,

$$k^2\,p + \lambda\,\partial_i\left(\frac{1}{\rho}\,\partial_i\,p\right) = 0\ , \tag{3.48}$$

where the expression in the parentheses is continuous. An equivalent L-S form of the last equation is

$$\left(\partial_i\partial_i + k^2\right)\left(\frac{1}{\rho}\,p\right) - k^2\left(\frac{1}{\rho} - \frac{1}{\lambda}\right)p - \partial_i\left[\left(\partial_i\,\frac{1}{\rho}\right)p\right] = 0\ . \tag{3.49}$$

We note two important features of this equation:

1. The equation is not really for the pressure p (which is continuous) but for p/ρ (which is discontinuous).

2. The potentially singular gradient of $1/\rho$ is multiplied by p (which is continuous).

Acoustics: L-S form of equations for the displacement. By taking the gradient of Eq.(3.47b) and eliminating the pressure p, we find an alternative second-order equation for the displacement, equivalent to the usual Lamé equation with $\mu = 0$,

$$k^2 u_i + \frac{1}{\rho} \partial_i \left(\lambda \partial_l u_l \right) = 0 \ . \tag{3.50}$$

Here, again, the expression in the parentheses is continuous. An equivalent L-S form of the last equation, analogous to Eq.(3.49), is then

$$\left(\partial_i \partial_j + \delta_{ij} k^2 \right) \left(\lambda u_j \right) - k^2 \left(\lambda - \rho \right) u_i - \partial_i \left[\left(\partial_j \lambda \right) u_j \right] = 0 \ . \tag{3.51}$$

Evidently, Eq.(3.51) is (apart from the different tensor structure) analogous to Eq.(3.49), under the replacements

$$\rho \longrightarrow \frac{1}{\lambda} \ , \qquad \lambda \longrightarrow \frac{1}{\rho} \ . \tag{3.52}$$

Eq.(3.51) has now properties analogous to those of of Eq.(3.49):

1. The unknown in the equation is not for the displacement u_i (which is continuous across interfaces) but rather λu_i (which is not continuous).

2. The possibly singular gradient of λ is multiplied by u_j, which is continuous.

Elasticity. There is, of course, no exact counterpart of Eq.(3.51) in the case of $\mu \neq 0$. However, a closely analogous equation is

$$\begin{aligned} \left(\partial_i \partial_j + \delta_{ij} k^2 \right) \left[\left(\lambda + 2\mu \right) u_j \right] - k^2 \left(\lambda + 2\mu - \rho \right) u_i - \partial_i \left[\left(\partial_j \lambda \right) u_j \right] \\ - \partial_j \left[2 \partial_i \left(\mu u_j \right) - \mu \left(\partial_i u_j + \partial_j u_i \right) \right] = 0 \ . \end{aligned} \tag{3.53}$$

The first three terms in this expression have the same form as the corresponding terms in Eq.(3.51), and the Lamé coefficient μ appears only in the last term.

4 Green functions in elasticity

As an initial step in formulating surface (boundary) integral equations we discuss here the Green functions of the Lameé equation for the displacement field in a general elastic medium. This form of the Green function will be used in the surface integral equations (Sec. 5).

On the other hand, in the Lippmann-Schwinger integral equations we will only need the Green function for the background medium – in our case, air.

For completeness, we give here a short derivation of the formulae for the Green function. We then represent it in the form most suitable for discretization of the integral equations, avoiding potential difficulties associated with its singular short-distance behavior.

The Green function of the Lamé equation. The Green function of Eq.(3.1) – a second-rank tensor – is defined by the equation

$$\left[\omega^2\,\rho\,\delta_{ij} + \partial_m\left(C_{imkj}\,\partial_k\right)\right]\;G_{jn}(\mathbf{r}) = -\,\delta_{in}\,\delta^3(\mathbf{r}) \tag{4.1}$$

and the radiation boundary conditions at infinity. Physically, the function $G_{jn}(\mathbf{r})$ is the displacement in the direction j generated by a point-like force located at the origin and acting in the direction n.

In the case of an infinite homogeneous medium the explicit form of the Green function (4.1) is known [2, 3], and can be derived as follows:

We represent the Green function G in terms of its Fourier transform $\widetilde{G}$,

$$\begin{aligned} G_{jn}(\mathbf{r}) &= \int \frac{\mathrm{d}^3 q}{(2\pi)^3}\,\mathrm{e}^{\mathrm{i}\,\mathbf{q}\cdot\mathbf{r}}\,\widetilde{G}_{jn}(\mathbf{q}) \\ &= \int \frac{\mathrm{d}^3 q}{(2\pi)^3}\,\mathrm{e}^{\mathrm{i}\,\mathbf{q}\cdot\mathbf{r}}\left[f_0(q)\,\delta_{jn} + f_2(q)\,q_j\,q_n\right]\ , \end{aligned} \tag{4.2}$$

where the Ansatz for $\widetilde{G}$ is based on the assumption of the medium isotropy. By substituting Eq.(4.2) in Eq.(4.1) and solving for f_0 and f_2 we find

$$\widetilde{G}_{ij}(\mathbf{q}) = \frac{1}{\mu}\left(\delta_{ij} - \frac{q_i\,q_j}{k_\mathrm{S}^2}\right)\frac{1}{q^2 - k_\mathrm{S}^2} + \frac{1}{\mu k_\mathrm{S}^2}\,\frac{q_i\,q_j}{q^2 - k_\mathrm{C}^2} \tag{4.3}$$

with

$$k_\mathrm{C}^2 = \omega^2\,\frac{\rho}{\lambda + 2\mu}\ , \qquad k_\mathrm{S}^2 = \omega^2\,\frac{\rho}{\mu}\ . \tag{4.4}$$

The two wave-numbers,

$$k_\mathrm{C} = \frac{\omega}{c_\mathrm{C}}\ , \qquad k_\mathrm{S} = \frac{\omega}{c_\mathrm{S}}\ , \tag{4.5}$$

correspond to two sound speeds,

$$c_\mathrm{C} = \sqrt{\frac{\lambda + 2\mu}{\rho}}\ , \qquad c_\mathrm{S} = \sqrt{\frac{\mu}{\rho}}\ , \tag{4.6}$$

for longitudinal (compressional) and transverse (shear) waves.

In the acoustics limit ($\mu \to 0$) (4.3) becomes

$$\widetilde{G}_{ij}(\mathbf{q})_{\mu=0} = -\,\frac{1}{\lambda k_\mathrm{C}^2}\left(\delta_{ij} - \frac{q_i\,q_j}{q^2 - k_\mathrm{C}^2}\right)\ . \tag{4.7}$$

The coordinate-space Green functions are then

$$G_{ij}(\mathbf{r}) = \frac{1}{\mu}\left(\delta_{ij} + \frac{1}{k_\mathrm{S}^2}\,\partial_i\,\partial_j\right) g_\mathrm{S}(r) - \frac{1}{\mu k_\mathrm{S}^2}\,\partial_i\,\partial_j\,g_\mathrm{C}(r)\ , \tag{4.8a}$$

and

$$G_{ij}(\mathbf{r})_{\mu=0} = -\,\frac{1}{\lambda k_\mathrm{C}^2}\left(\delta_{ij}\,\delta^3(\mathbf{r}) + \partial_i\,\partial_j\,g_\mathrm{C}(r)\right) \equiv -\,\frac{1}{\omega^2\,\rho}\left(\delta_{ij}\,\delta^3(\mathbf{r}) + \partial_i\,\partial_j\,g_\mathrm{C}(r)\right)\ , \tag{4.8b}$$

where

$$g_{\mathrm{C}}(r) = \frac{\mathrm{e}^{\mathrm{i}k_{\mathrm{C}}r}}{4\pi r} \equiv \frac{\mathrm{i}k_{\mathrm{C}}}{4\pi}\,\mathrm{h}_0^{(1)}(k_{\mathrm{C}}r) \ , \quad g_{\mathrm{S}}(r) = \frac{\mathrm{e}^{\mathrm{i}k_{\mathrm{S}}r}}{4\pi r} \equiv \frac{\mathrm{i}k_{\mathrm{S}}}{4\pi}\,\mathrm{h}_0^{(1)}(k_{\mathrm{S}}r) \ , \tag{4.9}$$

and the spherical Hankel functions of the first kind (Ref. [4], Ch. 10) are

$$\mathrm{h}_0^{(1)}(z) = -\frac{\mathrm{i}}{z}\,\mathrm{e}^{\mathrm{i}z} \ , \ \mathrm{h}_1^{(1)}(z) = -\frac{\mathrm{i}}{z^2}\,(1-\mathrm{i}z)\,\mathrm{e}^{\mathrm{i}z} \ , \ \mathrm{h}_2^{(1)}(z) = -\frac{\mathrm{i}}{z^3}\,(3-3\mathrm{i}z-z^2)\,\mathrm{e}^{\mathrm{i}z} \ . \tag{4.10}$$

By using relations between the Hankel functions and their derivatives, we find

$$\begin{aligned} \frac{1}{k^2}\,\partial_i\,\partial_j\,g(r) &\equiv \frac{1}{k^2}\left\{\delta_{ij}\,\frac{g'(r)}{r} + \hat{r}_i\,\hat{r}_j\left(g''(r) - \frac{g'(r)}{r}\right)\right\} \\ &= \frac{\mathrm{i}k}{12\pi}\left\{-\delta_{ij}\left[\mathrm{h}_0^{(1)}(kr) + \mathrm{h}_2^{(1)}(kr)\right] + 3\,\hat{r}_i\,\hat{r}_j\,\mathrm{h}_2^{(1)}(kr)\right\} \end{aligned} \tag{4.11}$$

and

$$\left(\delta_{ij} + \frac{1}{k^2}\,\partial_i\,\partial_j\right)g(r) = \frac{\mathrm{i}k}{12\pi}\left\{\delta_{ij}\left[2\,\mathrm{h}_0^{(1)}(kr) - \mathrm{h}_2^{(1)}(kr)\right] + 3\,\hat{r}_i\,\hat{r}_j\,\mathrm{h}_2^{(1)}(kr)\right\} \ . \tag{4.12}$$

Hence,

$$\begin{aligned} G_{ij}(\mathbf{r}) &= \frac{\mathrm{i}\,k_{\mathrm{C}}}{12\pi\,(\lambda+2\mu)}\,\left[\delta_{ij}\,\mathrm{h}_0^{(1)}(k_{\mathrm{C}}r) + (\delta_{ij} - 3\,\hat{r}_i\,\hat{r}_j)\,\mathrm{h}_2^{(1)}(k_{\mathrm{C}}r)\right] \\ &\quad - \frac{\mathrm{i}\,k_{\mathrm{S}}}{12\pi\,\mu}\,\left[-2\,\delta_{ij}\,\mathrm{h}_0^{(1)}(k_{\mathrm{S}}r) + (\delta_{ij} - 3\,\hat{r}_i\,\hat{r}_j)\,\mathrm{h}_2^{(1)}(k_{\mathrm{S}}r)\right] \ . \end{aligned} \tag{4.13}$$

In the limit $\mu \to 0$ Eq.(4.13) becomes

$$\begin{aligned} G_{ij}(\mathbf{r})_{\mu=0} &= \frac{\mathrm{i}\,k_{\mathrm{C}}}{12\pi\,\lambda}\,\left[\delta_{ij}\,\mathrm{h}_0^{(1)}(k_{\mathrm{C}}r) + (\delta_{ij} - 3\,\hat{r}_i\,\hat{r}_j)\,\mathrm{h}_2^{(1)}(k_{\mathrm{C}}r)\right] \\ &\quad - \frac{1}{\lambda k_{\mathrm{C}}^2}\,\delta_{ij}\,\delta^3(\mathbf{r}) \ , \end{aligned} \tag{4.14}$$

i.e., the shear-wave contribution reduces to a delta-function term.

A dyadic form of the the Green function. The Green function (4.8a) or (4.13) may be represented in a equivalent form involving dyadic derivatives. We first express the Green function and its derivatives in terms of the spherical Hankel functions of the first kind, (Ref. [4], Ch. 10),

$$\begin{aligned} g(\mathbf{r}) &\equiv \frac{\mathrm{e}^{\mathrm{ikr}}}{4\pi} = \frac{\mathrm{i}}{4\pi}\mathrm{h}_0^{(1)}(kr) \ , \\ g'(\mathbf{r}) &= \frac{\mathrm{i}k}{4\pi}\mathrm{h}_0^{(1)\prime}(kr) \ , \\ g''(\mathbf{r}) &= \frac{\mathrm{i}k^2}{4\pi}\mathrm{h}_0^{(1)\prime\prime}(kr) \ ; \end{aligned} \tag{4.15}$$

these expressions apply to both the Green functions (4.9). Hence,

$$
\begin{aligned}
\nabla_{\mathbf{r}} \otimes \nabla_{\mathbf{r}}\, g(r) &= \hat{I}\, \frac{g'(\mathbf{r})}{r} - \hat{\mathbf{r}} \otimes \hat{\mathbf{r}} \left[g''(r) - \frac{g'(r)}{r} \right] \\
&= \frac{\mathrm{i}k^2}{4\pi} \left\{ \hat{I}\, \frac{\mathrm{h}_0^{(1)\prime}(kr)}{kr} - \hat{\mathbf{r}} \otimes \hat{\mathbf{r}} \left[\mathrm{h}_0^{(1)\prime\prime}(kr) - \frac{\mathrm{h}_0^{(1)\prime}(kr)}{kr} \right] \right\} .
\end{aligned}
\tag{4.16}
$$

By using relations between the Hankel functions and their derivatives,

$$
\begin{aligned}
\mathrm{h}_0^{(1)\prime\prime}(z) &= \mathrm{h}_2^{(1)}(z) - \frac{\mathrm{h}_1^{(1)}(z)}{z} = \mathrm{h}_2^{(1)}(z) + \frac{\mathrm{h}_0^{(1)\prime}(z)}{z} \, , \\
\mathrm{h}_2^{(1)}(z) &= -\mathrm{h}_0^{(1)}(z) + \frac{3}{z}\mathrm{h}_1^{(1)}(z) = -\mathrm{h}_0^{(1)}(z) - \frac{3}{z}\mathrm{h}_0^{(1)\prime}(z) \\
&= -\frac{4\pi}{\mathrm{i}k^2} \left[k^2 g(r) + 3\, \frac{g'(r)}{r} \right] , \\
\mathrm{h}_2^{(1)}(z) + \mathrm{h}_0^{(1)}(z) &= \frac{3}{z}\mathrm{h}_1^{(1)}(z) = -\frac{4\pi}{\mathrm{i}k^2}\, \frac{3g'(r)}{r} \, , \\
\mathrm{h}_2^{(1)}(z) - 2\mathrm{h}_0^{(1)}(z) &= \mathrm{h}_0^{(1)}(z) + \frac{3}{z}\mathrm{h}_1^{(1)}(z) = -3\, \frac{4\pi}{\mathrm{i}k^2} \left[k^2 g(r) + \frac{g'(r)}{r} \right] ,
\end{aligned}
\tag{4.17}
$$

we obtain

$$
\begin{aligned}
\nabla_{\mathbf{r}} \otimes \nabla_{\mathbf{r}}\, g(r) &= \frac{\mathrm{i}k^2}{4\pi} \left[\frac{\mathrm{h}_0^{(1)\prime}(kr)}{kr} - \hat{\mathbf{r}} \otimes \hat{\mathbf{r}}\, \mathrm{h}_2^{(1)}(kr) \right] , \\
\hat{\mathbf{r}} \otimes \hat{\mathbf{r}}\, \mathrm{h}_2^{(1)}(kr) &= \frac{4\pi}{\mathrm{i}k^2} \left[\hat{I}\, \frac{g'(r)}{r} - \nabla_{\mathbf{r}} \otimes \nabla_{\mathbf{r}}\, g(r) \right] , \\
(\hat{I} - 3\, \hat{\mathbf{r}} \otimes \hat{\mathbf{r}})\, \mathrm{h}_2^{(1)}(kr) &= \mathrm{h}_2^{(1)}(kr) - 3\, \frac{4\pi}{\mathrm{i}k^2} \left[\hat{I}\, \frac{g'(r)}{r} - \nabla_{\mathbf{r}} \otimes \nabla_{\mathbf{r}}\, g(r) \right] \\
&= \frac{4\pi}{\mathrm{i}k^2} \left[-k^2 g(r) - 6\, \frac{g'(r)}{r} + \nabla_{\mathbf{r}} \otimes \nabla_{\mathbf{r}}\, g(r) \right] \\
\mathrm{h}_0^{(1)}(kr) + (\hat{I} - 3\, \hat{\mathbf{r}} \otimes \hat{\mathbf{r}})\, \mathrm{h}_2^{(1)}(kr) &= \frac{4\pi}{\mathrm{i}k^2} \left[-6\, \frac{g'(r)}{r} + 3\, \nabla_{\mathbf{r}} \otimes \nabla_{\mathbf{r}}\, g(r) \right] , \\
-2\, \mathrm{h}_0^{(1)}(kr) + (\hat{I} - 3\, \hat{\mathbf{r}} \otimes \hat{\mathbf{r}})\, \mathrm{h}_2^{(1)}(kr) &= \frac{4\pi}{\mathrm{i}k^2} \left[-3\, k^2 g(r) - 6\, \frac{g'(r)}{r} + 3\, \nabla_{\mathbf{r}} \otimes \nabla_{\mathbf{r}}\, g(r) \right] ,
\end{aligned}
\tag{4.18}
$$

and, finally,

$$
G(\mathbf{r}) = \frac{k_{\mathrm{C}}}{\lambda + 2\mu} \left(-2\, \frac{g_{\mathrm{C}}'(r)}{r} + \nabla_{\mathbf{r}} \otimes \nabla_{\mathbf{r}}\, g_{\mathrm{C}}(r) \right) - \frac{k_{\mathrm{S}}}{\mu} \left(-k_{\mathrm{S}}^2\, g_{\mathrm{S}}(r) - 2\, \frac{g_{\mathrm{S}}'(r)}{r} + \nabla_{\mathbf{r}} \otimes \nabla_{\mathbf{r}}\, g_{\mathrm{S}}(r) \right). \tag{4.19}
$$

An alternative form of the Green function: a reduced degree of singularity. In the same dyadic notation as above, we can also represent the Green function (4.8a) in the form

$$
G(\mathbf{r}) = \hat{I}\, C(r) + \nabla_{\mathbf{r}} \otimes \nabla_{\mathbf{r}}\, D(r) \, , \tag{4.20}
$$

with

$$C(r) := \frac{1}{\mu}\, g_{\mathrm{S}}(r)\ , \tag{4.21a}$$

$$D(r) := \frac{1}{\mu\, k_{\mathrm{S}}^2}\left[g_{\mathrm{S}}(r) - g_{\mathrm{C}}(r)\right]\ . \tag{4.21b}$$

The above representation exhibits an important property of the Green function (4.20): since the function $D(r)$ of Eq.(4.21b) is regular for $r \to 0$ (due to cancellation of the singularities in the two Green functions), the second term of the Green function (4.20) is also nonsingular, while, without the cancellation, it would have contained a $\sim 1/r^3$ singularity. The reduced degree of singularity is particularly important in the discretization of surface integral equations (Sec. 5).

5 Surface integral equations

We discuss here briefly the form of the surface boundary equations and their discretization, which is now being implemented in our solver.

5.1 Derivation of surface integral equations for scattering problems

Surface integral equations in elasticity can be derived from boundary-value problems involving boundary conditions defined on interfaces separating homogeneous material regions (for which unbounded-space Green functions, such a discussed in Sec. 4, are known).

The conventional procedure is to start with representation theorems expressing the fields in a region as an integral of an appropriate Green function and the values of the fields and (possibly) their derivatives on the boundary of the region; typically, such representations arise from the Green theorems and their generalizations. By imposing boundary conditions on the region-region interfaces, one can then obtain integral equations for the field values on those interfaces.

More precisely, the above approach is known as the "direct method". Other forms of integral equations can be obtained by "indirect methods" by postulating expressions (Ansätze) for the fields in terms of other sources supported on boundaries of the material regions.

In elasticity, a convenient form of the representation theorems [2, 5] involves the displacement field $\mathbf{u}(\mathbf{r})$ defined in a given domain Ω and on its boundary $\partial\Omega$, and the traction field $t(\mathbf{r})$ expressed in terms of the stress tensor τ, and defined on the (smooth) region boundary,

$$\mathbf{t}(\mathbf{r}) := \hat{\mathbf{n}}(\mathbf{r}) \cdot \tau(\mathbf{r})\ , \tag{5.1}$$

where $\hat{\mathbf{n}}$ is the exterior unit normal to $\partial\Omega$.

In addition to the second-rank tensor Green function G (Eq.(4.20)) for the displacement field, the representation theorems also require a third-rank tensor Green function Σ for the stress tensor; this quantity is defined as

$$\Sigma(\mathbf{r}) := \lambda\, \nabla \cdot\, G(\mathbf{r}) + \mu\left[\nabla\, G(\mathbf{r}) + G(\mathbf{r})\, \nabla\right]\ , \tag{5.2}$$

or, in index notation,

$$\Sigma_{ijk}(\mathbf{r}) := \lambda\, \delta_{ij}\, \partial_l\, G_{lk}(\mathbf{r}) + \mu \left[\partial_i\, G_{jk}(\mathbf{r}) + \partial_j\, G_{ik}(\mathbf{r})\right] \,, \tag{5.3}$$

i.e., Σ is related to the displacement Green function G in the same way as the stress tensor is related to the displacement field (Eq.(3.6)). We note that the Green function Σ_{ijk} is symmetric in its first two indices.

It is also convenient to introduce a second-rank tensor Green function Γ as a contraction of Σ with the normal vector,

$$\Gamma(\mathbf{r}, \mathbf{r}') := -\,\hat{\mathbf{n}}(\mathbf{r}') \cdot \Sigma(\mathbf{r} - \mathbf{r}'); \tag{5.4}$$

we note that $\Gamma(\mathbf{r}, \mathbf{r}')$ does not only depend on the relative distance $\mathbf{r} - \mathbf{r}'$, but rather on $\mathbf{r}$ and $\mathbf{r}'$ separately. In analogy to $\Gamma(\mathbf{r}, \mathbf{r}')$, we also write $G(\mathbf{r}, \mathbf{r}') \equiv G(\mathbf{r} - \mathbf{r}')$. Actually, the representation theorems involve the transpose Green functions, denoted by G^{T} and Γ^{T}.

It is of interest to note here that, since the displacement Green function (4.20) contains only an $\sim 1/r$ singularity, the stress-tensor Green function Γ may contain at most $\sim 1/r^2$, but not $\sim 1/r^3$ singularities. This fact facilitates discretization of the integral equations and computation of the matrix elements.

With the above definitions, the basic form of the representation theorem, applicable to a displacement field satisfying the homogeneous Lamé equation in the domain $\Omega \equiv \Omega_-$, is

$$\int_{\partial\Omega} \mathrm{d}^2 r' \left[\Gamma^{\mathrm{T}}_{\Omega_-}(\mathbf{t}, \mathbf{r}') \cdot \mathbf{u}(\mathbf{r}') + G^{\mathrm{T}}_{\Omega_-}(\mathbf{r}, \mathbf{r}') \cdot \mathbf{t}(\mathbf{r}')\right] = \begin{cases} \mathbf{u}(\mathbf{r}) & \text{for } \mathbf{r} \in \Omega_- \,, \\ \frac{1}{2}\mathbf{u}(\mathbf{r}) & \text{for } \mathbf{r} \in \partial\Omega \,, \\ \mathbf{0} & \text{for } \mathbf{r} \in \Omega_+ \,. \end{cases} \tag{5.5a}$$

In the second representation theorem the region Ω_- is interchanged with its complement $\Omega_+ := \mathbb{R}^3 \setminus \overline{\Omega}$,

$$\int_{\partial\Omega} \mathrm{d}^2 r' \left[\Gamma^{\mathrm{T}}_{\Omega_+}(\mathbf{t}, \mathbf{r}') \cdot \mathbf{u}(\mathbf{r}') + G^{\mathrm{T}}_{\Omega_+}(\mathbf{r}, \mathbf{r}') \cdot \mathbf{t}(\mathbf{r}')\right] = -\begin{cases} \mathbf{0} & \text{for } \mathbf{r} \in \Omega_- \,, \\ \frac{1}{2}\mathbf{u}(\mathbf{r}) & \text{for } \mathbf{r} \in \partial\Omega \,, \\ \mathbf{u}(\mathbf{r}) & \text{for } \mathbf{r} \in \Omega_+ \,. \end{cases} \tag{5.5b}$$

More precisely, the representation theorem (5.5b) assumes that the displacement field satisfies the Lamé equation in Ω_+ and the radiation boundary conditions at infinity; this fact implies that the displacement in Eq.(5.5b) is the scattered field, rather than the total field. It is also important to remember that the Green functions appearing in Eqs. (5.5a) and (5.5b) correspond to different regions, $\Omega_- \equiv \Omega$ and Ω_+. Finally, the expressions for $\mathbf{r} \in \partial\Omega$ have to be interpreted as improper integrals.

According to the general "direct method" procedure, the representation theorems (5.5) are now supplemented with the boundary conditions on an interface of two solids, which simply require continuity of the displacement and traction fields on the boundary $\partial\Omega$. It is now straightforward to obtain the set of integral equations for the unknown fields $\mathbf{u}$ and $\mathbf{t}$

on the boundary $\partial\Omega$,

$$\tfrac{1}{2}\,\mathbf{u}(\mathbf{r}) - \int_{\partial\Omega} \mathrm{d}^2 r' \left[\Gamma^{\mathrm{T}}_{\Omega_+}(\mathbf{t},\mathbf{r}')\cdot\mathbf{u}(\mathbf{r}') + G^{\mathrm{T}}_{\Omega_+}(\mathbf{r},\mathbf{r}')\cdot\mathbf{t}(\mathbf{r}')\right] = \mathbf{u}^{\mathrm{in}}(\mathbf{r})\ , \tag{5.6a}$$

$$\tfrac{1}{2}\,\mathbf{u}(\mathbf{r}) + \int_{\partial\Omega} \mathrm{d}^2 r' \left[\Gamma^{\mathrm{T}}_{\Omega_-}(\mathbf{t},\mathbf{r}')\cdot\mathbf{u}(\mathbf{r}') + G^{\mathrm{T}}_{\Omega_-}(\mathbf{r},\mathbf{r}')\cdot\mathbf{t}(\mathbf{r}')\right] = 0\ ; \tag{5.6b}$$

$\mathbf{u}^{\mathrm{in}}$ is here the incident field. Both equations hold at points $\mathbf{r} \in \partial\Omega$ and in both equations the unknowns are two three-dimensional vectors: the displacement and the traction fields $\mathbf{u}$ and $\mathbf{t}$.

The above form of surface integral equations applies to the simple case of a single domain Ω immersed in a background medium. It can be generalized in a rather straightforward way to the case of multiple regions (domains) separated by interfaces. The general form of the resulting system of equations is given in Section 2, Eqs. (2.1).

5.2 Basis functions and discretization of surface integral equations

In order to solve the surface integral equations (5.5) numerically, it is necessary to make assumptions on the discretization of the solution, i.e., on the trial basis functions, and on the test basis functions.

In our implementation we use a discretization uniquely determined by our choice of discretization in the volumetric equations (discussed in detail in Sec. 6). We also use, similarly to the volumetric problem, the Galerkin discretization, i.e., identical trial and testing basis functions.

In the volumetric problem we assume the displacement field is expanded in piecewise linear basis functions supported on sets of tetrahedra. In the corresponding surface problem we use, therefore, restrictions of these basis functions to the facets of the tetrahedra to their boundary facets (triangles). The resulting surface basis functions are piecewise linear vector basis functions describing the components of the displacement field $\mathbf{u}$. By symmetry between the displacement and traction fields in the integral equations, we assume analogous linear basis functions for the components of $\mathbf{t}$.

According to the above criteria, we specify the basis functions as follows:

For each vertex $\mathbf{v}_\alpha$ of the surface mesh we define three vector basis functions, denoted $\boldsymbol{\psi}_\alpha(\mathbf{r})$, representing displacements in the x, y, and z directions. Correspondingly, the index α refers to the vertex and the direction, $\alpha = (\mathbf{v}_\alpha, m)$, $m = 1, 2, 3$ (or $m = x, y, z$).

Each such function, $\boldsymbol{\psi}_\alpha(\mathbf{r})$, is associated with a vertex $\mathbf{v}_\alpha$ and supported on a set of triangles (facets) f_α sharing that vertex. We parametrize the basis function as

$$\boldsymbol{\psi}_\alpha(\mathbf{r}) \equiv \boldsymbol{\psi}_{\mathbf{v}_\alpha,m}(\mathbf{r}) = \mathbf{e}_m\,\phi_{\mathbf{v}_\alpha}(\mathbf{r})\ , \tag{5.7}$$

where $\mathbf{e}_m$ is the unit vector along the m-the axis, and $\phi_{\mathbf{v}_\alpha}$ is a scalar basis function defined by

$$\phi_\alpha(\mathbf{r}) \equiv \phi_{\mathbf{v}_\alpha}(\mathbf{r}) = \sum_{f_\alpha \in \mathcal{F}_\alpha} \phi_{\mathbf{v}_\alpha, f_\alpha}(\mathbf{r})\ , \tag{5.8}$$

where the sum is taken over the set $\mathcal{F}_\alpha$ of all facets f_α sharing the vertex $\mathbf{v}_\alpha$. Further, each of the linear functions $\phi_{\mathbf{v}_\alpha, f_\alpha}(\mathbf{r})$, supported on the facet f_α, is uniquely defined by setting

its value to unity at $\mathbf{r} = \mathbf{v}_\alpha$ and to zero at the remaining vertices of the facet. An explicit expression is

$$\phi_{\mathbf{v}_\alpha,\, f_\alpha}(\mathbf{r}) = \left[1 - \frac{1}{h_{\mathbf{v}_\alpha,\, f_\alpha}}\, \hat{\mathbf{n}}_{\mathbf{v}_\alpha,\, f_\alpha} \cdot (\mathbf{r} - \mathbf{v}_\alpha)\right] \chi_{f_\alpha}(\mathbf{r}) \ , \tag{5.9}$$

where $\chi_{f_\alpha}(\mathbf{r})$ is the characteristic function of the facet f_α, $\hat{\mathbf{n}}_{\mathbf{v}_\alpha,\, f_\alpha}$ is the unit outer normal to the facet edge opposite the vertex $\mathbf{v}_\alpha$, and $h_{\mathbf{v}_\alpha,\, f_\alpha}$ is the facet height relative to that edge. Components of the basis function $\boldsymbol{\psi}_\alpha$ are then

$$\psi^i_\alpha(\mathbf{r}) \equiv \psi^i_{\mathbf{v}_\alpha,m}(\mathbf{r}) = \delta_{mi}\, \phi_{\mathbf{v}_\alpha}(\mathbf{r}) \ . \tag{5.10}$$

As follows from the construction, the scalar and vectorial basis functions (5.8) and (5.7) are two-dimensional analogues (actually, restrictions) of the piecewise linear basis functions supported on tetrahedra and used in the volumetric formulation (Secs. 6.1.1 and 6.1.2). The advantage of this discretization scheme is that the solutions of the surface and volumetric equations can be directly compared with one another.

5.3 Structure of the stiffness matrix and computation of matrix elements

Galerkin discretization of the integral equations (5.6) results in two types of matrix elements,

$$A^G_{\alpha\beta} = \int_{\mathcal{F}_\alpha} \mathrm{d}^2 r_1 \int_{\mathcal{F}_\beta} \mathrm{d}^2 r_2\, \boldsymbol{\psi}_\alpha(\mathbf{r}_1) \cdot G^{\mathrm{T}}(\mathbf{r}_1, \mathbf{r}_2) \cdot \boldsymbol{\psi}_\beta(\mathbf{r}_2) \tag{5.11a}$$

and

$$A^\Gamma_{\alpha\beta} = \int_{\mathcal{F}_\alpha} \mathrm{d}^2 r_1 \int_{\mathcal{F}_\beta} \mathrm{d}^2 r_2\, \boldsymbol{\psi}_\alpha(\mathbf{r}_1) \cdot \Gamma^{\mathrm{T}}(\mathbf{r}_1, \mathbf{r}_2) \cdot \boldsymbol{\psi}_\beta(\mathbf{r}_2) \ , \tag{5.11b}$$

with the Green functions corresponding to one of the regions in question. The integrals are taken here over sets of facets, $\mathcal{F}_\alpha$ and $\mathcal{F}_\beta$, sharing the vertices $\mathbf{v}_\alpha$ and $\mathbf{v}_\beta$; therefore, they can be expressed as sums of integrals taken over pairs of facets f_α and f_β.

We give now some examples of more explicit expressions for the matrix elements (5.11b). They are still comparatively simple relative to those for the volumetric equations, discussed in detail in Sec. 6. The procedures of simplifying the matrix elements are similar in both cases and involve, mostly, integration by parts and using the defining equations for the Green functions.

We consider below the more involved matrix element $A^\Gamma_{\alpha\beta}$, in which we set $\alpha = (\mathbf{v}_\alpha, m)$ and $\beta = (\mathbf{v}_\beta, n)$. A contribution to this matrix element from a pair of facets f_α and f_β has

the form

$$\begin{aligned}
&A^{\Gamma}_{\alpha\beta}(f_\alpha, f_\beta) \equiv A^{\Gamma}_{\mathbf{v}_\alpha,m;\,\mathbf{v}_\beta,n}(f_\alpha, f_\beta) \\
&= -\int_{f_\alpha} \mathrm{d}^2 r_1 \int_{f_\beta} \mathrm{d}^2 r_2 \, \phi_{\mathbf{v}_\alpha,\,f_\alpha}(\mathbf{r}_1)\, \mathbf{e}_m \cdot \Gamma^{\mathrm{T}}(\mathbf{r}_1, \mathbf{r}_2) \cdot \mathbf{e}_n \, \phi_{\mathbf{v}_\beta,\,f_\beta}(\mathbf{r}_2) \\
&= -\int_{f_\alpha} \mathrm{d}^2 r_1 \int_{f_\beta} \mathrm{d}^2 r_2 \, \phi_{\mathbf{v}_\alpha,\,f_\alpha}(\mathbf{r}_1)\, \Sigma_{inm}(\mathbf{r}_1 - \mathbf{r}_2)\, n_i(\mathbf{r}_2)\, \phi_{\mathbf{v}_\beta,\,f_\beta}(\mathbf{r}_2) \\
&= -\int_{f_\alpha} \mathrm{d}^2 r_1 \int_{f_\beta} \mathrm{d}^2 r_2 \, \phi_{\mathbf{v}_\alpha,\,f_\alpha}(\mathbf{r}_1)\, \{\lambda\, \delta_{in}\, \partial_l\, G_{lm}(\mathbf{r}_1 - \mathbf{r}_2) \\
&\qquad\qquad + \mu \left[\partial_i\, G_{nm}(\mathbf{r}_1 - \mathbf{r}_2) + \partial_n\, G_{im}(\mathbf{r}_1 - \mathbf{r}_2)\right]\} \\
&\qquad\qquad\qquad n_i(\mathbf{r}_2)\, \phi_{\mathbf{v}_\beta,\,f_\beta}(\mathbf{r}_2) \; .
\end{aligned} \tag{5.12}$$

Further manipulations of the matrix element involve substitution of the representation of the displacement Green function (4.20), e.g.,

$$G_{lm}(\mathbf{r}_1 - \mathbf{r}_2) = \delta_{lm}\, C(|\mathbf{r}_1 - \mathbf{r}_2|) + \partial_l\, \partial_m\, D(|\mathbf{r}_1 - \mathbf{r}_2|) \; . \tag{5.13}$$

One of the resulting terms, involving the Lamé coefficient λ and the function D, becomes then

$$-\lambda \int_{f_\alpha} \mathrm{d}^2 r_1 \int_{f_\beta} \mathrm{d}^2 r_2 \, \phi_{\mathbf{v}_\alpha,\,f_\alpha}(\mathbf{r}_1)\, \partial_l\, \partial_l\, \partial_m\, D(\mathbf{r}_1 - \mathbf{r}_2)\, n_n(\mathbf{r}_2)\, \phi_{\mathbf{v}_\beta,\,f_\beta}(\mathbf{r}_2) \; . \tag{5.14}$$

This expression can be further simplified by using the relation

$$\partial_l\, \partial_l\, D(\mathbf{r}) \equiv \nabla^2 D(\mathbf{r}) = \frac{1}{\lambda + 2\mu}\, g_{\mathrm{C}}(r) - \frac{1}{\mu}\, g_{\mathrm{S}}(r) \; , \tag{5.15}$$

following from Eq.(4.21b) and the defining equations for the Green functions g_{C} and g_{S}. Finally, integration by parts transforms Eq.(5.14) into

$$\lambda \int_{f_\alpha} \mathrm{d}^2 r_1 \int_{f_\beta} \mathrm{d}^2 r_2 \, \partial_m\, \phi_{\mathbf{v}_\alpha,\,f_\alpha}(\mathbf{r}_1) \left[\frac{1}{\lambda + 2\mu}\, g_{\mathrm{C}}(\mathbf{r}_1 - \mathbf{r}_2) - \frac{1}{\mu}\, g_{\mathrm{S}}(\mathbf{r}_1 - \mathbf{r}_2)\right] n_n(\mathbf{r}_2)\, \phi_{\mathbf{v}_\beta,\,f_\beta}(\mathbf{r}_2) \; . \tag{5.16}$$

Since the basis function $\phi_{\mathbf{v}_\alpha,\,f_\alpha}$ is linear on the facet f_α, its gradient is the sum of a constant on that facet and of linear delta-functions supported on its boundaries. In the sum over the facets contributing to the full matrix element $A^{\Gamma}_{\alpha\beta}$ the contributions of delta-functions from adjacent facets cancel. This cancellation is complete in the problem of a single domain Ω, for which $\partial\Omega$ is a closed surface; however, delta-function contributions from facet edges may remain for more complex topologies with several material regions.

Other terms in the matrix element can be treated in a similar way. For instance, the term inolving λ and the function $C(r)$ is very similar to Eq.(5.16),

$$\frac{\lambda}{\mu} \int_{f_\alpha} \mathrm{d}^2 r_1 \int_{f_\beta} \mathrm{d}^2 r_2 \, \partial_m\, \phi_{\mathbf{v}_\alpha,\,f_\alpha}(\mathbf{r}_1)\, g_{\mathrm{S}}(\mathbf{r}_1 - \mathbf{r}_2)\, n_n(\mathbf{r}_2)\, \phi_{\mathbf{v}_\beta,\,f_\beta}(\mathbf{r}_2) \; . \tag{5.17}$$

The more involved term proportional to the Lamé coefficient μ is

$$\begin{aligned}
&\int_{f_\alpha} \mathrm{d}^2 r_1 \int_{f_\beta} \mathrm{d}^2 r_2 \, \partial_i \, \phi_{\mathbf{v}_\alpha, f_\alpha}(\mathbf{r}_1) \, \delta_{mn} \, g_{\mathrm{C}}(\mathbf{r}_1 - \mathbf{r}_2) \, n_i(\mathbf{r}_2) \, \phi_{\mathbf{v}_\beta, f_\beta}(\mathbf{r}_2) \\
&+ \int_{f_\alpha} \mathrm{d}^2 r_1 \int_{f_\beta} \mathrm{d}^2 r_2 \, \partial_n \, \phi_{\mathbf{v}_\alpha, f_\alpha}(\mathbf{r}_1) \, g_{\mathrm{C}}(\mathbf{r}_1 - \mathbf{r}_2) \, n_m(\mathbf{r}_2) \, \phi_{\mathbf{v}_\beta, f_\beta}(\mathbf{r}_2) \\
&- \frac{2}{k_{\mathrm{S}}^2} \int_{f_\alpha} \mathrm{d}^2 r_1 \int_{f_\beta} \mathrm{d}^2 r_2 \, \partial_i \, \phi_{\mathbf{v}_\alpha, f_\alpha}(\mathbf{r}_1) \, \partial_m \, \partial_n \left[g_{\mathrm{C}}(\mathbf{r}_1 - \mathbf{r}_2) - g_{\mathrm{S}}(\mathbf{r}_1 - \mathbf{r}_2) \right] n_i(\mathbf{r}_2) \, \phi_{\mathbf{v}_\beta, f_\beta}(\mathbf{r}_2) \ .
\end{aligned} \tag{5.18}$$

Although the third term in this expression involves two derivatives, the result is well defined, since the difference of the Green functions appearing there is nonsingular.

6 Volumetric integral equations

We describe here two formulations of the volumetric (L-S) integral equations, based, respectively, on first- and second-order differential equations of elasticity. In addition, we recast the more conventional of the equations into forms better suited to handling high-contrast problems.

On the level of the differential and integral equations themselves, these two approaches are exactly equivalent. They differ, however, in the choice of the unknowns and in the treatment of the material properties, hence in discretization aspects.

In order to allow direct comparison of the two formulations, we use in both cases the same basis functions; Therefore, we discuss the basis functions at the beginning of this Section.

6.1 Basis functions

Before deriving integral equations following from the differential equations analyzed above, we introduce basis functions which will be used in the discretization.

6.1.1 Piecewise linear scalar basis functions

As an underlying form of basis functions we will be assuming piecewise linear scalar functions supported on sets of tetrahedra sharing a common vertex, and interpolating between 1 at that vertex and 0 at the remaining vertices of the set of tetrahedra. We represent such a function ϕ_α as

$$\phi_\alpha(\mathbf{r}) \equiv \phi_{\mathbf{v}_\alpha}(\mathbf{r}) = \sum_{t_\alpha \in \mathcal{T}_\alpha} \phi_{\mathbf{v}_\alpha, t_\alpha}(\mathbf{r}) \ , \tag{6.1}$$

where the sum is taken over the set $\mathcal{T}_\alpha$ of all tetrahedra t_α sharing the vertex $\mathbf{v}_\alpha$, and each of the linear functions $\phi_{\mathbf{v}_\alpha, t_\alpha}(\mathbf{r})$, supported on the tetrahedron t_α, is defined to be unity at $\mathbf{r} = \mathbf{v}_\alpha$ and zero at the remaining vertices of t_α. An explicit expression is

$$\phi_{\mathbf{v}_\alpha, t_\alpha}(\mathbf{r}) = \left[1 - \frac{1}{h_{\mathbf{v}_\alpha, t_\alpha}} \, \hat{\mathbf{n}}_{\mathbf{v}_\alpha, t_\alpha} \cdot (\mathbf{r} - \mathbf{v}_\alpha) \right] \chi_{t_\alpha}(\mathbf{r}) \ , \tag{6.2}$$

where $\chi_{t_\alpha}(\mathbf{r})$ is the characteristic function of the tetrahedron t_α, $\hat{\mathbf{n}}_{\mathbf{v}_\alpha, t_\alpha}$ is the unit outer normal to the tetrahedron face opposite the vertex $\mathbf{v}_\alpha$, and $h_{\mathbf{v}_\alpha, t_\alpha}$ is the tetrahedron height relative to that face. When using such basis functions we assume, as before, that the material parameters are constant on the tetrahedra.

First derivatives of the basis function ϕ_α. The basis function ϕ_α is, obviously, continuous and differentiable (except for interfaces between the tetrahedra, where the derivatives do not exist). However, the individual functions $\phi_{\mathbf{v}_\alpha, t_\alpha}$ are not continuous, because they characteristic functions are not; therefore, their gradients are constant inside the tetrahedra, but involve also delta-functions concentrated on the interfaces between the tetrahedra in the set $\mathcal{T}_\alpha$. Explicitly,

$$\nabla \phi_{\mathbf{v}_\alpha, t_\alpha}(\mathbf{r}) = -\frac{1}{h_{\mathbf{v}_\alpha, t_\alpha}} \hat{\mathbf{n}}_{\mathbf{v}_\alpha, t_\alpha} \chi_{t_\alpha}(\mathbf{r}) - \phi_{\mathbf{v}_\alpha, t_\alpha}(\mathbf{r}) \, \hat{\mathbf{n}}(\mathbf{r}) \, \delta_{\partial t_\alpha}(\mathbf{r}) \tag{6.3a}$$

$$= -\frac{1}{h_{\mathbf{v}_\alpha, t_\alpha}} \hat{\mathbf{n}}_{\mathbf{v}_\alpha, t_\alpha} \chi_{t_\alpha}(\mathbf{r}) - \sum_{f_\alpha \in \partial t_\alpha} \phi_{\mathbf{v}_\alpha, f_\alpha}(\mathbf{r}) \, \hat{\mathbf{n}}_{f_\alpha, t_\alpha} \, \delta_{f_\alpha}(\mathbf{r}) \ . \tag{6.3b}$$

Here, in Eq.(6.3a), $\delta_{\partial t_\alpha}$ is the delta function concentrated on the tetrahedron boundary, and $\hat{\mathbf{n}}(\mathbf{r})$ is the outer unit normal to that boundary. In Eq.(6.3b), $f_\alpha \in \partial t_\alpha$ are faces of the tetrahedron t_α, $\hat{\mathbf{n}}_{f_\alpha, t_\alpha}$ is the unit normal to the face f_α in the direction out of the tetrahedron t_α, and $\phi_{\mathbf{v}_\alpha, f_\alpha}$ is the basis function $\phi_{\mathbf{v}_\alpha, t_\alpha}$ restricted to the face f_α. Because of continuity of ϕ_α, the function $\phi_{\mathbf{v}_\alpha, f_\alpha}$ is well defined; it is linear, and interpolates between 1 at the vertex $\mathbf{v}_\alpha$ and 0 at the remaining vertices of the face.

The delta-function contribution to the gradient (6.3) vanishes on the exterior boundary of the set $\mathcal{T}_\alpha$ of the tetrahedra (because the basis function $\phi_{\mathbf{v}_\alpha, t_\alpha}$ vanishes there), but it is nonzero on the other faces.

The delta-function terms cancel pairwise in the sum over the tetrahedra $t_\alpha \in \mathcal{T}_\alpha$, hence the gradient of function $\phi_{\mathbf{v}_\alpha}$ is regular, consistently with the fact that the function $\phi_{\mathbf{v}_\alpha}$ itself (given by the sum of (6.1)) is continuous.

However, the delta functions may give nonzero contributions if the vertex $\mathbf{v}_\alpha$ is located on the object boundary $\partial\Omega$, and thus some of the facets f_α are not interfaces but rather the boundary facets of the object.

Second derivatives of the basis function ϕ_α. Several expressions for matrix elements (e.g., (6.59d) and (6.59e) in the following) involve second derivatives of the basis function $\phi_{\mathbf{v}_\alpha}$, which are delta functions and derivatives of delta functions, concentrated on the interfaces of the tetrahedra in the set $\mathcal{T}_\alpha$ (i.e., tetrahedra sharing the vertex $\mathbf{v}_\alpha$). From the expression (6.3b) for the first derivatives we obtain, for each of the basis functions supported on a tetrahedron t_α,

$$\begin{aligned} \partial^m \partial^i \phi_{\mathbf{v}_\alpha, t_\alpha}(\mathbf{r}) = \frac{1}{h_{\mathbf{v}_\alpha, t_\alpha}} \sum_{f_\alpha \in \partial t_\alpha} & \left(\hat{n}^m_{\mathbf{v}_\alpha, t_\alpha} \hat{n}^i_{f_\alpha} + \hat{n}^i_{\mathbf{v}_\alpha, t_\alpha} \hat{n}^m_{f_\alpha} \right) \delta_{f_\alpha}(\mathbf{r}) \\ - \sum_{f_\alpha \in \partial t_\alpha} & \hat{n}^m_{f_\alpha} \hat{n}^i_{f_\alpha} \phi_{\mathbf{v}_\alpha, f_\alpha}(\mathbf{r}) \, \delta'_{f_\alpha}(\hat{\mathbf{n}}_{f_\alpha}, \mathbf{r}) \ . \end{aligned} \tag{6.4}$$

The notation used here for the delta function derivative actually means

$$\delta'_{f_\alpha}(\hat{\mathbf{n}}_{f_\alpha},\mathbf{r}) = \chi_{f_\alpha}(\mathbf{r}_{f_\alpha})\,\delta'_{f_\alpha}(\hat{\mathbf{n}}_{f_\alpha}\cdot\mathbf{r}) \ , \tag{6.5}$$

where $\mathbf{r}_{f_\alpha}$ is the projection of $\mathbf{r}$ on the facet f_α along the direction $\hat{\mathbf{n}}_{f_\alpha}$. The derivatives of delta function contribute only for facets f_α having $\mathbf{v}_\alpha$ as one of their vertices, since on the facet opposite the vertex $\mathbf{v}_\alpha$ the function $\phi_{\mathbf{v}_\alpha,f_\alpha}(\mathbf{r})$ vanishes.

In the double derivatives of the basis function $\phi_{\mathbf{v}_\alpha}(\mathbf{r})$ (Eq.(6.1)) each ***interior*** facet $f_\alpha\in\mathcal{F}_\alpha$ contributes to two adjacent tetrahedra, and the derivatives of the delta functions cancel, since $\delta'_{f_\alpha}(\hat{\mathbf{n}}_{f_\alpha},\mathbf{r})+\delta'_{f_\alpha}(-\hat{\mathbf{n}}_{f_\alpha},\mathbf{r})=0$. For boundary facets ($f_\alpha\in\partial\Omega$), however, the derivatives of the delta functions remain; hence

$$\begin{aligned}
\partial^m\,\partial^i\,\phi_{\mathbf{v}_\alpha}(\mathbf{r}) &= \sum_{t_\alpha\in\mathcal{T}_\alpha}\frac{1}{h_{\mathbf{v}_\alpha,t_\alpha}}\sum_{f_\alpha\in\partial t_\alpha}\left(\hat{n}^m_{\mathbf{v}_\alpha,t_\alpha}\,\hat{n}^i_{f_\alpha}+\hat{n}^i_{\mathbf{v}_\alpha,t_\alpha}\,\hat{n}^m_{f_\alpha}\right)\,\delta_{f_\alpha}(\mathbf{r}) \\
&\quad-\sum_{f_\alpha\in\mathcal{F}_\alpha\cap\partial\Omega}\hat{n}^m_{f_\alpha}\,\hat{n}^i_{f_\alpha}\,\phi_{\mathbf{v}_\alpha,f_\alpha}(\mathbf{r})\,\delta'_{f_\alpha}(\hat{\mathbf{n}}_{f_\alpha},\mathbf{r}) \qquad (6.6\text{a})\\
&= -\sum_{f_\alpha\in\mathcal{T}_\alpha}\Bigg[\frac{1}{h_{\mathbf{v}_\alpha,t_\alpha+}}\left(\hat{n}^m_{\mathbf{v}_\alpha,t_\alpha+}\,\hat{n}^i_{f_\alpha}+\hat{n}^i_{\mathbf{v}_\alpha,t_\alpha+}\,\hat{n}^m_{f_\alpha}\right) \\
&\qquad\qquad-\frac{1}{h_{\mathbf{v}_\alpha,t_\alpha-}}\left(\hat{n}^m_{\mathbf{v}_\alpha,t_\alpha-}\,\hat{n}^i_{f_\alpha}+\hat{n}^i_{\mathbf{v}_\alpha,t_\alpha-}\,\hat{n}^m_{f_\alpha}\right)\Bigg] \\
&\quad-\sum_{f_\alpha\in\mathcal{F}_\alpha\cap\partial\Omega}\hat{n}^m_{f_\alpha}\,\hat{n}^i_{f_\alpha}\,\phi_{\mathbf{v}_\alpha,f_\alpha}(\mathbf{r})\,\delta'_{f_\alpha}(\hat{\mathbf{n}}_{f_\alpha},\mathbf{r}) \ . \qquad (6.6\text{b})
\end{aligned}$$

The second form of this expression is obtained by grouping contributions from each facet f_α and denoting by $t_\alpha+$ and $t_\alpha-$ tetrahedra on the positive and negative sides of the facet (according to the direction of the normal $\hat{\mathbf{n}}_{f_\alpha}$). The sum in Eq.(6.6b), however, is taken over ***all*** facets f_α belonging to ***any tetrahedron*** in the set $\mathcal{T}_\alpha$, not only over facets $f_\alpha\in\mathcal{F}_\alpha$ sharing the ***vertex*** $\mathbf{v}_\alpha$; we indicate this by writing $f_\alpha\in\mathcal{T}_\alpha$. If the facet f_α is an exterior facet of the set $\mathcal{T}_\alpha$, i.e., $f_\alpha\in\partial\mathcal{T}_\alpha$, the contribution of the tetrahedron $t_\alpha+$ is absent.

A simple geometrical analysis shows that, for interfaces f_α, the linear combination of the normals $\hat{\mathbf{n}}_{\mathbf{v}_\alpha,t_\alpha+}$ and $\hat{\mathbf{n}}_{\mathbf{v}_\alpha,t_\alpha-}$ in Eq.(6.6b) is proportional to $\hat{\mathbf{n}}_{f_\alpha}$,

$$\frac{\hat{\mathbf{n}}_{\mathbf{v}_\alpha,t_\alpha+}}{h_{\mathbf{v}_\alpha,t_\alpha+}}-\frac{\hat{\mathbf{n}}_{\mathbf{v}_\alpha,t_\alpha-}}{h_{\mathbf{v}_\alpha,t_\alpha-}}\sim\mathbf{n}_{f_\alpha} \ . \tag{6.7}$$

Therefore, Eq.(6.6b) can be written as

$$\begin{aligned}
\partial^m\,\partial^i\,\phi_{\mathbf{v}_\alpha}(\mathbf{r}) &= -\,2\sum_{f_\alpha\in\mathcal{F}_\alpha}\left(\frac{\hat{\mathbf{n}}_{\mathbf{v}_\alpha,t_\alpha+}\cdot\hat{\mathbf{n}}_{f_\alpha}}{h_{\mathbf{v}_\alpha,t_\alpha+}}-\frac{\hat{\mathbf{n}}_{\mathbf{v}_\alpha,t_\alpha-}\cdot\hat{\mathbf{n}}_{f_\alpha}}{h_{\mathbf{v}_\alpha,t_\alpha-}}\right)\hat{n}^m_{f_\alpha}\,\hat{n}^i_{f_\alpha}\,\delta_{f_\alpha}(\mathbf{r}) \\
&\quad+\,2\sum_{f_\alpha\in\partial\mathcal{T}_\alpha}\frac{1}{h_{\mathbf{v}_\alpha,t_\alpha}}\,\hat{n}^m_{f_\alpha}\,\hat{n}^i_{f_\alpha}\,\delta_{f_\alpha}(\mathbf{r}) \qquad (6.8)\\
&\quad-\sum_{f_\alpha\in\mathcal{F}_\alpha\cap\partial\Omega}\hat{n}^m_{f_\alpha}\,\hat{n}^i_{f_\alpha}\,\delta'_{f_\alpha}(\hat{\mathbf{n}}_{f_\alpha},\mathbf{r})\,\phi_{\mathbf{v}_\alpha,f_\alpha}(\mathbf{r}) \ .
\end{aligned}$$

We have separated here contributions from the facets sharing the vertex $\mathbf{v}_\alpha$ and the facets on the boundary $\partial\mathcal{T}_\alpha$ of the set of tetrahedra. In the latter contribution $h_{\mathbf{v}_\alpha,t_\alpha}$ is the height of the tetrahedron adjacent to the facet f_α, measured from the vertex $\mathbf{v}_\alpha$.

6.1.2 Piecewise linear vector basis functions

In the following we consider linear vector-valued basis functions $\boldsymbol{\psi}_\alpha(\mathbf{r})$ associated with vertices and supported on sets of tetrahedra sharing the given vertex. For each vertex $\mathbf{v}_\alpha$ we define three vector basis functions representing displacements in the x, y, and z directions; the index α in $\boldsymbol{\psi}_\alpha$ refers thus to the vertex and the direction, $\alpha = (\mathbf{v}_\alpha, m)$, $m = 1, 2, 3$ (i.e., $m = x, y, z$).

We parametrize these functions $\boldsymbol{\psi}_\alpha$ as

$$\boldsymbol{\psi}_\alpha(\mathbf{r}) \equiv \boldsymbol{\psi}_{\mathbf{v}_\alpha,m}(\mathbf{r}) = \mathbf{e}_m\, \phi_{\mathbf{v}_\alpha}(\mathbf{r}) \ , \tag{6.9}$$

where $\mathbf{e}_m$ is the unit vector along the m-the axis, and $\phi_{\mathbf{v}_\alpha}$ is the scalar basis function defined by Eq.(6.1). Components of the basis function $\boldsymbol{\psi}_\alpha$ (as appearing in Eqs. (6.58)) are then

$$\psi^i_\alpha(\mathbf{r}) \equiv \psi^i_{\mathbf{v}_\alpha,m}(\mathbf{r}) = \delta_{mi}\, \phi_{\mathbf{v}_\alpha}(\mathbf{r}) \ . \tag{6.10}$$

The derivatives of the basis functions appearing in Eqs. (6.58) represent either the pressure or the strain tensor,

$$\Psi_{\mathbf{v}_\alpha,m}(\mathbf{r}) \equiv \partial^i\, \psi^i_{\mathbf{v}_\alpha,m}(\mathbf{r}) = \partial^m\, \phi_{\mathbf{v}_\alpha}(\mathbf{r}) \tag{6.11}$$

or

$$\begin{aligned} \Psi^{ij}_{\mathbf{v}_\alpha,m}(\mathbf{r}) &\equiv \tfrac{1}{2}\, \left[\partial^i\, \psi^j_{\mathbf{v}_\alpha,m}(\mathbf{r}) + \partial^j\, \psi^i_{\mathbf{v}_\alpha,m}(\mathbf{r})\right] \\ &= \tfrac{1}{2}\, \Big[\delta_{mi}\, \partial^j\, \phi_{\mathbf{v}_\alpha}(\mathbf{r}) + \delta_{mj}\, \partial^i\, \phi_{\mathbf{v}_\alpha}(\mathbf{r})\Big] \ ; \end{aligned} \tag{6.12}$$

these expressions are valid, of course, for any (not only linear) scalar basis functions ϕ. We note that the divergence of the basis function representing displacement in the direction m is, actually, a derivative of the scalar basis function in that direction.

6.2 Integral equations in first-order formulation

General structure of the L-S equations. The system of equations (3.29) with a prescribed source $\mathcal{S}$ has the form

$$\mathcal{K}\,\mathcal{F} \equiv (\mathcal{D} + \mathcal{V})\,\mathcal{F} = -\,\mathcal{S} \ , \tag{6.13}$$

where the source is assumed to act in the space of traceless symmetric tensor fields σ,

$$\mathcal{I}\,\mathcal{S} = \mathcal{S} \ . \tag{6.14}$$

It can be now verified, with the use of projection properties (3.39), (6.14), (3.42), and (3.43), as well as the definition (3.34) of the Green function, that Eq.(6.13) can be represented as the L-S equation

$$(\mathcal{I} - \mathcal{G}\,\mathcal{V})\,\mathcal{F} = \mathcal{G}\,\mathcal{S} =: \mathcal{F}^{\text{in}}, \tag{6.15}$$

where $\mathcal{F}^{\text{in}}$ is the incident field.

It follows immediately from Eq.(3.35) that some blocks of the Green function are identically zero,

$$\mathcal{G} = \left[\begin{array}{c:c:c} \mathcal{G}^{\mathrm{vv}} & \mathcal{G}^{\mathrm{vp}} & \mathcal{G}^{\mathrm{v}\sigma} \\ \hdashline \mathcal{G}^{\mathrm{pv}} & \mathcal{G}^{\mathrm{pp}} & \mathcal{G}^{\mathrm{p}\sigma} \\ \hdashline 0 & 0 & \mathcal{G}^{\sigma\sigma} \end{array}\right] . \tag{6.16}$$

Therefore, the kernel $\mathcal{G}\,\mathcal{V}$ appearing in the L-S equation (6.15),

$$\mathcal{W} := \mathcal{G}\,\mathcal{V} = \left[\begin{array}{c:c:c} \mathcal{G}^{\mathrm{vv}} & \mathcal{G}^{\mathrm{vp}} & \mathcal{G}^{\mathrm{v}\sigma} \\ \hdashline \mathcal{G}^{\mathrm{pv}} & \mathcal{G}^{\mathrm{pp}} & \mathcal{G}^{\mathrm{p}\sigma} \\ \hdashline 0 & 0 & \mathcal{G}^{\sigma\sigma} \end{array}\right] \left[\begin{array}{c:c:c} \mathcal{V}^{\mathrm{vv}} & 0 & 0 \\ \hdashline 0 & \mathcal{V}^{\mathrm{pp}} & 0 \\ \hdashline \mathcal{V}^{\sigma\mathrm{v}} & 0 & 0 \end{array}\right] = \left[\begin{array}{c:c:c} \mathcal{W}^{\mathrm{vv}} & \mathcal{W}^{\mathrm{vp}} & 0 \\ \hdashline \mathcal{W}^{\mathrm{pv}} & \mathcal{W}^{\mathrm{pp}} & 0 \\ \hdashline \mathcal{W}^{\sigma\mathrm{v}} & 0 & 0 \end{array}\right] , \tag{6.17}$$

also exhibits a number of zero blocks.

Evaluation of the Green function. The system of equations (3.35) for the Green function components can be easily solved in terms of the Fourier transforms

$$\mathcal{G}^{ab}_{\dots}(\mathbf{r}) = \int \frac{\mathrm{d}^3 q}{(2\pi)^3}\, \mathrm{e}^{\mathrm{i}\,\mathbf{q}\cdot\mathbf{r}}\, \widetilde{\mathcal{G}}^{ab}_{\dots}(\mathbf{q}) , \qquad a, b = \mathrm{v}, \mathrm{p}, \sigma . \tag{6.18}$$

Eq.(3.35) becomes then

$$\begin{aligned} &\left[\begin{array}{c:c:c} \mathrm{i}\,k\,\delta_{ik} & -\mathrm{i}\,q_i & \mathrm{i}\,\delta_{ik}\,q_l \\ \hdashline -\mathrm{i}\,q_k & \mathrm{i}\,k & 0 \\ \hdashline 0 & 0 & \mathrm{i}\,k\,\delta_{ik}\,\delta_{jl} \end{array}\right] \left[\begin{array}{c:c:c} \widetilde{\mathcal{G}}^{\mathrm{vv}}_{km} & \widetilde{\mathcal{G}}^{\mathrm{vp}}_{k} & \widetilde{\mathcal{G}}^{\mathrm{v}\sigma}_{kmn} \\ \hdashline \widetilde{\mathcal{G}}^{\mathrm{pv}}_{m} & \widetilde{\mathcal{G}}^{\mathrm{pp}} & \widetilde{\mathcal{G}}^{\mathrm{p}\sigma}_{mn} \\ \hdashline \widetilde{\mathcal{G}}^{\sigma\mathrm{v}}_{klm} & \widetilde{\mathcal{G}}^{\sigma\mathrm{p}}_{kl} & \widetilde{\mathcal{G}}^{\sigma\sigma}_{klmn} \end{array}\right] (\mathbf{q}) \\ &\qquad\qquad = - \left[\begin{array}{c:c:c} \delta_{im} & 0 & 0 \\ \hdashline 0 & 1 & 0 \\ \hdashline 0 & 0 & \Delta_{ijmn} \end{array}\right] . \end{aligned} \tag{6.19}$$

By considering the last row of equations in the system we find immediately

$$\widetilde{\mathcal{G}}^{\sigma\mathrm{v}}_{klm}(\mathbf{q}) = 0 , \tag{6.20a}$$

$$\widetilde{\mathcal{G}}^{\sigma\mathrm{p}}_{kl}(\mathbf{q}) = 0 , \tag{6.20b}$$

$$\widetilde{\mathcal{G}}^{\sigma\sigma}_{klmn}(\mathbf{q}) = \frac{\mathrm{i}}{k}\,\Delta_{klmn} . \tag{6.20c}$$

After substituting these expressions in the remaining equations, we obtain

$$\mathrm{i}\,k\,\widetilde{\mathcal{G}}^{\mathrm{vv}}_{im}(\mathbf{q}) - \mathrm{i}\,q_i\,\widetilde{\mathcal{G}}^{\mathrm{pv}}_{m}(\mathbf{q}) = -\,\delta_{im}\ , \tag{6.21a}$$

$$\mathrm{i}\,k\,\widetilde{\mathcal{G}}^{\mathrm{vp}}_{i}(\mathbf{q}) - \mathrm{i}\,q_i\,\widetilde{\mathcal{G}}^{\mathrm{pp}}(\mathbf{q}) = 0\ , \tag{6.21b}$$

$$\mathrm{i}\,k\,\widetilde{\mathcal{G}}^{\mathrm{v}\sigma}_{imn}(\mathbf{q}) - \mathrm{i}\,q_i\,\widetilde{\mathcal{G}}^{\mathrm{p}\sigma}_{mn}(\mathbf{q}) + \mathrm{i}\,q_l\,\frac{\mathrm{i}}{k}\,\Delta_{ilmn} = 0\ , \tag{6.21c}$$

$$-\,\mathrm{i}\,q_k\,\widetilde{\mathcal{G}}^{\mathrm{vv}}_{km}(\mathbf{q}) + \mathrm{i}\,k\,\widetilde{\mathcal{G}}^{\mathrm{pv}}_{m}(\mathbf{q}) = 0\ , \tag{6.21d}$$

$$-\,\mathrm{i}\,q_k\,\widetilde{\mathcal{G}}^{\mathrm{vp}}_{k}(\mathbf{q}) + \mathrm{i}\,k\,\widetilde{\mathcal{G}}^{\mathrm{pp}}(\mathbf{q}) = -\,1\ , \tag{6.21e}$$

$$-\,\mathrm{i}\,q_k\,\widetilde{\mathcal{G}}^{\mathrm{v}\sigma}_{kmn}(\mathbf{q}) + \mathrm{i}\,k\,\widetilde{\mathcal{G}}^{\mathrm{p}\sigma}_{mn}(\mathbf{q}) = 0\ . \tag{6.21f}$$

The subsystem of equations (6.21a), (6.21b), (6.21d), and (6.21e) is associated with the acoustic problem, described by the fields $\mathbf{v}$ and p. It can be easily solved by substituting the Ansätze based on rotational invariance,

$$\widetilde{\mathcal{G}}^{\mathrm{vv}}_{km}(\mathbf{q}) = a(q)\,\delta_{km} + b(q)\,q_k\,q_m\ , \tag{6.22a}$$

$$\widetilde{\mathcal{G}}^{\mathrm{vp}}_{k}(\mathbf{q}) = \widetilde{\mathcal{G}}^{\mathrm{pv}}_{k}(\mathbf{q}) = c(q)\,q_k\ , \tag{6.22b}$$

$$\widetilde{\mathcal{G}}^{\mathrm{pp}}(\mathbf{q}) = d(q)\ . \tag{6.22c}$$

The solution is then

$$\widetilde{\mathcal{G}}^{\mathrm{vv}}_{km}(\mathbf{q}) = \frac{\mathrm{i}}{k}\left(\delta_{km} - \frac{q_k\,q_m}{\mathbf{q}^2 - k^2}\right)\ , \tag{6.23a}$$

$$\widetilde{\mathcal{G}}^{\mathrm{vp}}_{k}(\mathbf{q}) = \widetilde{\mathcal{G}}^{\mathrm{pv}}_{k}(\mathbf{q}) = \frac{-\mathrm{i}\,q_k}{\mathbf{q}^2 - k^2}\ , \tag{6.23b}$$

$$\widetilde{\mathcal{G}}^{\mathrm{pp}}(\mathbf{q}) = \frac{-\mathrm{i}\,k}{\mathbf{q}^2 - k^2}\ . \tag{6.23c}$$

Out of the remaining equations, Eq.(6.21f) allows us to express $\widetilde{\mathcal{G}}^{\mathrm{p}\sigma}$ in terms of $\widetilde{\mathcal{G}}^{\mathrm{v}\sigma}$,

$$\widetilde{\mathcal{G}}^{\mathrm{p}\sigma}_{mn}(\mathbf{q}) = \frac{q_l}{k}\,\widetilde{\mathcal{G}}^{\mathrm{v}\sigma}_{lmn}(\mathbf{q})\ , \tag{6.24}$$

and the last equation to be solved, (6.21c), becomes

$$\begin{aligned}(k^2\,\delta_{il} - q_i\,q_l)\,\widetilde{\mathcal{G}}^{\mathrm{v}\sigma}_{lmn}(\mathbf{q}) &= -\,\mathrm{i}\,q_l\,\Delta_{ilmn} \\ &\equiv -\,\tfrac{\mathrm{i}}{2}\,(\delta_{im}\,q_n + \delta_{in}\,q_m - \tfrac{2}{3}\,q_i\,\delta_{mn})\ .\end{aligned} \tag{6.25}$$

By substituting here the Ansatz

$$\widetilde{\mathcal{G}}^{\mathrm{v}\sigma}_{lmn}(\mathbf{q}) = A(q)\,\Delta_{klmn}\,q_k + B(q)\,\Delta_{ijmn}\,q_i\,q_j\,q_l \tag{6.26}$$

we find, finally, solutions for $\widetilde{\mathcal{G}}^{\mathrm{v}\sigma}$ and then $\widetilde{\mathcal{G}}^{\mathrm{p}\sigma}$ as

$$\widetilde{\mathcal{G}}^{\mathrm{v}\sigma}_{lmn}(\mathbf{q}) = -\,\frac{\mathrm{i}}{k^2}\left(\Delta_{klmn}\,q_k - \frac{\Delta_{ijmn}\,q_i\,q_j\,q_l}{\mathbf{q}^2 - k^2}\right)\ , \tag{6.27a}$$

$$\widetilde{\mathcal{G}}^{\mathrm{p}\sigma}_{mn}(\mathbf{q}) = \frac{\mathrm{i}}{k}\,\frac{\Delta_{ijmn}\,q_i\,q_j}{\mathbf{q}^2 - k^2}\ . \tag{6.27b}$$

These expressions are manifestly symmetric and traceless in the indices m, n.

The structure of the Green function matrix and its blocks (Eqs. (6.23), (6.20c), and (6.27)) can be summarized as

$$
\begin{aligned}
\widetilde{\mathcal{G}}(\mathbf{q}) &= \left[\begin{array}{c:c:c}
\widetilde{\mathcal{G}}^{\mathrm{vv}}_{km} & \widetilde{\mathcal{G}}^{\mathrm{vp}}_{k} & \widetilde{\mathcal{G}}^{\mathrm{v}\sigma}_{kmn} \\ \hdashline
\widetilde{\mathcal{G}}^{\mathrm{pv}}_{m} & \widetilde{\mathcal{G}}^{\mathrm{pp}} & \widetilde{\mathcal{G}}^{\mathrm{p}\sigma}_{mn} \\ \hdashline
\widetilde{\mathcal{G}}^{\sigma\mathrm{v}}_{klm} & \widetilde{\mathcal{G}}^{\sigma\mathrm{p}}_{kl} & \widetilde{\mathcal{G}}^{\sigma\sigma}_{klmn}
\end{array}\right](\mathbf{q}) \\
&= \left[\begin{array}{c:c:c}
\dfrac{\mathrm{i}}{k}\left(\delta_{km} - \dfrac{q_k\, q_m}{\mathbf{q}^2 - k^2}\right) & \dfrac{-\mathrm{i}\, q_k}{\mathbf{q}^2 - k^2} & -\dfrac{\mathrm{i}}{k^2}\left(\Delta_{klmn}\, q_l - \dfrac{\Delta_{ijmn}\, q_i\, q_j\, q_k}{\mathbf{q}^2 - k^2}\right) \\ \hdashline
\dfrac{-\mathrm{i}\, q_m}{\mathbf{q}^2 - k^2} & \dfrac{-\mathrm{i}\, k}{\mathbf{q}^2 - k^2} & \dfrac{\mathrm{i}}{k}\, \dfrac{\Delta_{ijmn}\, q_i\, q_j}{\mathbf{q}^2 - k^2} \\ \hdashline
0 & 0 & \dfrac{\mathrm{i}}{k}\, \Delta_{klmn}
\end{array}\right] .
\end{aligned}
\tag{6.28}
$$

The Green function in coordinate space. Fourier transformation (6.18) of the Green function operator (3.41) back to the coordinate space involves just the substitutions $q_k \to -\mathrm{i}\, \partial_k$ and the usual Helmholtz-equation Green function

$$
g(\mathbf{r}) \equiv g(r) := \int \frac{\mathrm{d}^3 q}{(2\pi)^3}\, \mathrm{e}^{\mathrm{i}\,\mathbf{q}\cdot\mathbf{r}}\, \frac{1}{\mathbf{q}^2 - k^2 - \mathrm{i}\,0} = \frac{\mathrm{e}^{\mathrm{i}kr}}{4\pi r}
\tag{6.29}
$$

(with $r := |\mathbf{r}|$), satisfying the equation

$$
(\nabla^2 + k^2)\, g(\mathbf{r}) = -\,\delta^3(\mathbf{r})
\tag{6.30}
$$

and the radiation boundary condition. Hence,

$$
\begin{aligned}
\mathcal{G}(\mathbf{r}) &= \left[\begin{array}{c:c:c}
\mathcal{G}^{\mathrm{vv}}_{km} & \mathcal{G}^{\mathrm{vp}}_{k} & \mathcal{G}^{\mathrm{v}\sigma}_{kmn} \\ \hdashline
\mathcal{G}^{\mathrm{pv}}_{m} & \mathcal{G}^{\mathrm{pp}} & \mathcal{G}^{\mathrm{p}\sigma}_{mn} \\ \hdashline
\mathcal{G}^{\sigma\mathrm{v}}_{klm} & \mathcal{G}^{\sigma\mathrm{p}}_{kl} & \mathcal{G}^{\sigma\sigma}_{klmn}
\end{array}\right](\mathbf{r}) \\
&= \left[\begin{array}{c:c:c}
\begin{array}{l}\dfrac{\mathrm{i}}{k}\left[\delta_{km}\, \delta^3(\mathbf{r})\right. \\ \qquad \left. +\, \partial_k \partial_m\, g(\mathbf{r})\right]\end{array} & -\,\partial_k\, g(\mathbf{r}) & \begin{array}{l}-\dfrac{1}{k^2}\left[\Delta_{klmn}\, \partial_l\, \delta^3(\mathbf{r})\right. \\ \qquad \left. +\, \Delta_{ijmn}\, \partial_i \partial_j \partial_k\, g(\mathbf{r})\right]\end{array} \\ \hdashline
-\,\partial_m\, g(\mathbf{r}) & -\mathrm{i}\, k\, g(\mathbf{r}) & -\dfrac{\mathrm{i}}{k}\, \Delta_{ijmn}\, \partial_i \partial_j\, g(\mathbf{r}) \\ \hdashline
0 & 0 & \dfrac{\mathrm{i}}{k}\, \Delta_{klmn}\, \delta^3(\mathbf{r})
\end{array}\right] .
\end{aligned}
\tag{6.31}
$$

By using the definitions (3.36) and (6.30) of the tensor Δ and the Green function g, one can further simplify the blocks $\mathcal{G}^{\mathrm{v}\sigma}$ and $\mathcal{G}^{\mathrm{p}\sigma}$ to

$$
\mathcal{G}^{\mathrm{v}\sigma}_{kmn}(\mathbf{r}) = -\,k^{-2}\left[\tfrac{1}{2}\left(\delta_{km}\, \partial_n + \delta_{kn}\, \partial_m\right) \delta^3(\mathbf{r}) + \partial_k\, g_{mn}(\mathbf{r})\right] ,
\tag{6.32a}
$$

$$
\mathcal{G}^{\mathrm{p}\sigma}_{mn}(\mathbf{r}) = -\,\mathrm{i}\, k^{-1}\left(\tfrac{1}{3}\, \delta_{mn}\, \delta^3(\mathbf{r}) + g_{mn}\right) ,
\tag{6.32b}
$$

where we defined, for convenience, an auxiliary symmetric Green function

$$g_{mn}(\mathbf{r}) := \left(\tfrac{1}{3}\,\delta_{mn}\,k^2 + \partial_m\partial_n\right) g(\mathbf{r}) \ . \tag{6.33}$$

The L-S integral equations. An explicit form of the integral equations (reflecting the structure of Eq.(6.17)) is

$$\begin{aligned}
\rho(\mathbf{r})\,v_i(\mathbf{r}) &+ \int \mathrm{d}^3r'\,\left[\partial_i\partial_m\,g(\mathbf{r}-\mathbf{r}')\right]\left[\rho(\mathbf{r}')-1\right] v_m(\mathbf{r}') \\
&+ \frac{1}{k^2}\int \mathrm{d}^3r'\,\Big\{\left[\partial_m\,\delta^3(\mathbf{r}-\mathbf{r}')\right]\mu(\mathbf{r}')\left[\partial'_i\,v_m(\mathbf{r}')+\partial'_m\,v_i(\mathbf{r}')\right] \\
&\qquad\qquad + \left[\partial_i\,g_{mn}(\mathbf{r}-\mathbf{r}')\right] 2\mu(\mathbf{r}')\,\partial'_m\,v_n(\mathbf{r}')\Big\} \\
&+ \mathrm{i}k\int \mathrm{d}^3r'\,\left[\partial_i\,g(\mathbf{r}-\mathbf{r}')\right]\left[\varphi(\mathbf{r}')-1\right] p(\mathbf{r}') \\
&= v_i^{\mathrm{in}}(\mathbf{r}) \ ,
\end{aligned} \tag{6.34a}$$

$$\begin{aligned}
p(\mathbf{r}) &- k^2\int \mathrm{d}^3r'\,g(\mathbf{r}-\mathbf{r}')\left[\varphi(\mathbf{r}')-1\right] p(\mathbf{r}') \\
&+ \frac{2\mathrm{i}}{3k}\,\mu(\mathbf{r})\,\partial_m\,v_m(\mathbf{r}) + \frac{\mathrm{i}}{k}\int \mathrm{d}^3r'\,g_{mn}(\mathbf{r}-\mathbf{r}')\,2\mu(\mathbf{r}')\,\partial'_m\,v_n(\mathbf{r}') \\
&= p^{\mathrm{in}}(\mathbf{r}) \ ,
\end{aligned} \tag{6.34b}$$

$$\begin{aligned}
\sigma_{ij}(\mathbf{r}) &- \frac{\mathrm{i}}{k}\,\mu(\mathbf{r})\left[\partial_i\,v_j(\mathbf{r})+\partial_j\,v_i(\mathbf{r})-\tfrac{2}{3}\,\delta_{ij}\,\partial_m\,v_m(\mathbf{r})\right] \\
&= \sigma_{ij}^{\mathrm{in}}(\mathbf{r}) \ .
\end{aligned} \tag{6.34c}$$

In particular, because of the vanishing third column of the kernel $\mathcal{W}$ of Eq.(6.17), the stress tensor σ does not appear at all in the first two equations, (6.34a) and (6.34b). These equations can be thus solved for $\mathbf{v}$ and p, and, if desired, the stress tensor can be evaluated by using Eq.(6.34c), which just reproduces Eq.(3.29c).

The integral equations (6.34) above are written in the form assuming $\rho_0 = \lambda_0 = 1$. After

reintroducing these parameters, equations (6.34) take the final form

$$
\begin{aligned}
\frac{\rho(\mathbf{r})}{\rho_0}\, v_i(\mathbf{r}) &+ \int \mathrm{d}^3 r' \,\big(\partial_i \partial_m\, g(\mathbf{r}-\mathbf{r}')\big) \left(\frac{\rho(\mathbf{r}')}{\rho_0} - 1\right) v_m(\mathbf{r}') \\
&+ \frac{1}{k^2}\, \partial_m \left[\frac{\mu(\mathbf{r})}{\lambda_0} \big(\partial_i\, v_m(\mathbf{r}) + \partial_m\, v_i(\mathbf{r})\big)\right] \\
&+ \frac{1}{k^2} \int \mathrm{d}^3 r' \,\big(\partial_i\, g_{mn}(\mathbf{r}-\mathbf{r}')\big)\, \frac{2\mu(\mathbf{r}')}{\lambda_0}\, \partial'_m\, v_n(\mathbf{r}') \\
&+ \frac{\mathrm{i}\, k}{\lambda_0} \int \mathrm{d}^3 r' \,\big(\partial_i\, g(\mathbf{r}-\mathbf{r}')\big) \big(\varphi(\mathbf{r}') - 1\big)\, p(\mathbf{r}') \\
&= v_i^{\mathrm{in}}(\mathbf{r}) \;,
\end{aligned}
\tag{6.35a}
$$

$$
\begin{aligned}
p(\mathbf{r}) - k^2 &\int \mathrm{d}^3 r' \, g(\mathbf{r}-\mathbf{r}') \big(\varphi(\mathbf{r}') - 1\big)\, p(\mathbf{r}') \\
&+ \frac{2\mathrm{i}}{3k}\, \frac{\mu(\mathbf{r})}{\lambda_0}\, \partial_m\, v_m(\mathbf{r}) + \frac{\mathrm{i}}{k} \int \mathrm{d}^3 r' \, g_{mn}(\mathbf{r}-\mathbf{r}')\, \frac{2\mu(\mathbf{r}')}{\lambda_0}\, \partial'_m\, v_n(\mathbf{r}') \\
&= p^{\mathrm{in}}(\mathbf{r}) \;,
\end{aligned}
\tag{6.35b}
$$

$$
\begin{aligned}
\sigma_{ij}(\mathbf{r}) - \frac{\mathrm{i}}{k}\, \frac{\mu(\mathbf{r})}{\lambda_0} &\big[\partial_i\, v_j(\mathbf{r}) + \partial_j\, v_i(\mathbf{r}) - \tfrac{2}{3}\, \delta_{ij}\, \partial_m\, v_m(\mathbf{r})\big] \\
&= \sigma_{ij}^{\mathrm{in}}(\mathbf{r}) \;.
\end{aligned}
\tag{6.35c}
$$

6.2.1 Matrix elements: general expressions

We discretize the L-S equations (6.35) by using the Galerkin method, in terms of vector and scalar basis functions $\boldsymbol{\psi}_\alpha$ and ϕ_α for the fields $\mathbf{v}$ and p. The resulting stiffness matrix takes then the form

$$
A = \left[\begin{array}{c:c} A^{\mathrm{vv}} & A^{\mathrm{vp}} \\ \hdashline A^{\mathrm{pv}} & A^{\mathrm{pp}} \end{array}\right] \;,
\tag{6.36}
$$

with the blocks

$$A^{\mathrm{vv}}_{\alpha\beta} = \int \mathrm{d}^3 r\, \psi^i_\alpha(\mathbf{r})\, \frac{\rho(\mathbf{r})}{\rho_0}\, \psi^i_\beta(\mathbf{r})$$
$$- \int \mathrm{d}^3 r_1 \int \mathrm{d}^3 r_2 \left(\partial^i_1 \psi^i_\alpha(\mathbf{r}_1)\right) \left(\partial^j_1\, g(\mathbf{r}_1 - \mathbf{r}_2)\right) \left(\frac{\rho(\mathbf{r}_2)}{\rho_0} - 1\right) \psi^j_\beta(\mathbf{r}_2)$$
$$- \frac{1}{k^2} \int \mathrm{d}^3 r \left(\partial^i \psi^j_\alpha(\mathbf{r})\right) \frac{\mu(\mathbf{r})}{\lambda_0} \left(\partial^i \psi^j_\beta(\mathbf{r}) + \partial^j \psi^i_\beta(\mathbf{r})\right)$$
$$- \frac{2}{k^2} \int \mathrm{d}^3 r_1 \int \mathrm{d}^3 r_2 \left(\partial^i_1 \psi^i_\alpha(\mathbf{r}_1)\right) g_{kl}(\mathbf{r}_1 - \mathbf{r}_2)\, \frac{\mu(\mathbf{r}_2)}{\lambda_0} \left(\partial^k_2 \psi^l_\beta(\mathbf{r}_2)\right) , \tag{6.37a}$$
$$A^{\mathrm{vp}}_{\alpha\beta} = -\frac{\mathrm{i}\, k}{\lambda_0} \int \mathrm{d}^3 r_1 \int \mathrm{d}^3 r_2 \left(\partial^i_1 \psi^i_\alpha(\mathbf{r}_1)\right) g(\mathbf{r}_1 - \mathbf{r}_2) \left(\varphi(\mathbf{r}_2) - 1\right) \phi_\beta(\mathbf{r}_2) , \tag{6.37b}$$
$$A^{\mathrm{pv}}_{\alpha\beta} = \frac{2\mathrm{i}}{3k} \int \mathrm{d}^3 r\, \phi_\alpha(\mathbf{r})\, \mu(\mathbf{r}) \left(\partial^j \psi^j_\beta(\mathbf{r})\right) \tag{6.37c}$$
$$+ \frac{2\mathrm{i}}{k} \int \mathrm{d}^3 r_1 \int \mathrm{d}^3 r_2\, \phi_\alpha(\mathbf{r}_1)\, g_{kl}(\mathbf{r}_1 - \mathbf{r}_2)\, \mu(\mathbf{r}_2) \left(\partial^k_2 \psi^l_\beta(\mathbf{r}_2)\right) , \tag{6.37d}$$
$$A^{\mathrm{pp}}_{\alpha\beta} = -k^2 \int \mathrm{d}^3 r_1 \int \mathrm{d}^3 r_2\, \phi_\alpha(\mathbf{r}_1)\, g(\mathbf{r}_1 - \mathbf{r}_2) \left(\varphi(\mathbf{r}_2) - 1\right) \phi_\beta(\mathbf{r}_2) . \tag{6.37e}$$

6.2.2 Matrix elements with composite linear basis functions

In the following we assume piecewise linear vector and scalar basis functions, as described in Sections 6.1.2 and 6.1.1. By expressing the vector basis functions in terms of the scalar ones (Eq.(6.9)), we can represent Eqs. (6.37) as

$$A^{\mathrm{vv}}_{\mathbf{v}_\alpha,m;\mathbf{v}_\beta,n} = \delta_{mn} \int \mathrm{d}^3 r\, \frac{\rho(\mathbf{r})}{\rho_0}\, \phi_{\mathbf{v}_\alpha}(\mathbf{r})\, \phi_{\mathbf{v}_\beta}(\mathbf{r})$$
$$- \int \mathrm{d}^3 r_1 \int \mathrm{d}^3 r_2 \left(\partial^m_1 \phi_{\mathbf{v}_\alpha}(\mathbf{r}_1)\right) \left(\partial^n_1\, g(\mathbf{r}_1 - \mathbf{r}_2)\right) \left(\frac{\rho(\mathbf{r}_2)}{\rho_0} - 1\right) \phi_{\mathbf{v}_\beta}(\mathbf{r}_2)$$
$$- \frac{1}{k^2} \int \mathrm{d}^3 r\, \frac{\mu(\mathbf{r})}{\lambda_0} \left[\delta_{mn} \left(\partial^j \phi_{\mathbf{v}_\alpha}(\mathbf{r})\right) \left(\partial^j \phi_{\mathbf{v}_\beta}(\mathbf{r})\right) + \left(\partial^n \phi_{\mathbf{v}_\alpha}(\mathbf{r})\right) \left(\partial^m \phi_{\mathbf{v}_\beta}(\mathbf{r})\right)\right]$$
$$- \frac{2}{k^2} \int \mathrm{d}^3 r_1 \int \mathrm{d}^3 r_2 \left(\partial^m_1 \phi_{\mathbf{v}_\alpha}(\mathbf{r}_1)\right) g_{kn}(\mathbf{r}_1 - \mathbf{r}_2)\, \frac{\mu(\mathbf{r}_2)}{\lambda_0} \left(\partial^k_2 \phi_{\mathbf{v}_\beta}(\mathbf{r}_2)\right) , \tag{6.38a}$$
$$A^{\mathrm{vp}}_{\mathbf{v}_\alpha,m;\mathbf{v}_\beta} = -\frac{\mathrm{i}\, k}{\lambda_0} \int \mathrm{d}^3 r_1 \int \mathrm{d}^3 r_2 \left(\partial^m_1 \phi_{\mathbf{v}_\alpha}(\mathbf{r}_1)\right) g(\mathbf{r}_1 - \mathbf{r}_2) \left(\varphi(\mathbf{r}_2) - 1\right) \phi_{\mathbf{v}_\beta}(\mathbf{r}_2) , \tag{6.38b}$$
$$A^{\mathrm{pv}}_{\mathbf{v}_\alpha;\mathbf{v}_\beta,n} = \frac{2\mathrm{i}}{3k} \int \mathrm{d}^3 r\, \phi_{\mathbf{v}_\alpha}(\mathbf{r})\, \mu(\mathbf{r}) \left(\partial^n \phi_{\mathbf{v}_\beta}(\mathbf{r})\right)$$
$$+ \frac{2\mathrm{i}}{k} \int \mathrm{d}^3 r_1 \int \mathrm{d}^3 r_2\, \phi_{\mathbf{v}_\alpha}(\mathbf{r}_1)\, g_{kn}(\mathbf{r}_1 - \mathbf{r}_2)\, \mu(\mathbf{r}_2) \left(\partial^k_2 \phi_{\mathbf{v}_\beta}(\mathbf{r}_2)\right) , \tag{6.38c}$$
$$A^{\mathrm{pp}}_{\mathbf{v}_\alpha;\mathbf{v}_\beta} = -k^2 \int \mathrm{d}^3 r_1 \int \mathrm{d}^3 r_2\, \phi_{\mathbf{v}_\alpha}(\mathbf{r}_1)\, g(\mathbf{r}_1 - \mathbf{r}_2) \left(\varphi(\mathbf{r}_2) - 1\right) \phi_{\mathbf{v}_\beta}(\mathbf{r}_2) ; \tag{6.38d}$$

as before, vector basis functions are labeled by pairs of indices $(\mathbf{v}_\alpha, m)$ or $(\mathbf{v}_\beta, n)$, representing the vertex and the Cartesian component of the vector, and the scalar basis functions are indexed by the vertices only.

6.2.3 Matrix elements with elementary linear basis functions

As before, we now have to express, in Eqs. (6.38), the "composite" basis functions (supported on sets of tetrahedra) in terms of "elementary" basis functions supported on individual tetrahedra or facets. By using the relations of Section 6.1.1 we find the displacement-displacement matrix elements in the form

$$
\begin{aligned}
A^{\mathrm{vv}}_{\mathbf{v}_\alpha,m;\mathbf{v}_\beta,n} = \delta_{mn} & \sum_{t_\alpha\in\mathcal{T}_\alpha} \frac{\rho(t_\alpha)}{\rho_0} \int_{t_\alpha} \mathrm{d}^3 r\, \phi_{\mathbf{v}_\alpha,t_\alpha}(\mathbf{r})\, \phi_{\mathbf{v}_\beta,t_\beta}(\mathbf{r}) && \text{(6.39a)}\\
&- k^{-2} \sum_{t_\alpha\in\mathcal{T}_\alpha} \frac{\mu(t_\alpha)}{\lambda_0}\, v_\alpha\, \frac{1}{h_{\mathbf{v}_\alpha,t_\alpha}}\, \frac{1}{h_{\mathbf{v}_\beta,t_\alpha}} \\
&\qquad \Big[\delta_{mn}\, \hat{n}^i_{\mathbf{v}_\alpha,t_\alpha}\, \hat{n}^i_{\mathbf{v}_\beta,t_\alpha} + \hat{n}^n_{\mathbf{v}_\alpha,t_\alpha}\, \hat{n}^m_{\mathbf{v}_\beta,t_\alpha} - \tfrac{2}{3}\, \hat{n}^m_{\mathbf{v}_\alpha,t_\alpha}\, \hat{n}^n_{\mathbf{v}_\beta,t_\alpha}\Big] && \text{(6.39b)}\\
&+ \sum_{t_\alpha\in\mathcal{T}_\alpha} \sum_{t_\beta\in\mathcal{T}_\beta} \left(\frac{\rho(t_\beta)}{\rho_0} - 1\right) \frac{1}{h_{\mathbf{v}_\alpha,t_\alpha}}\, \hat{n}^m_{\mathbf{v}_\alpha,t_\alpha} \\
&\qquad \int_{t_\alpha} \mathrm{d}^3 r_1 \int_{t_\beta} \mathrm{d}^3 r_2\, \phi_{\mathbf{v}_\beta,t_\beta}(\mathbf{r}_1)\, \big(\partial^n_1\, g(\mathbf{r}_1-\mathbf{r}_2)\big) && \text{(6.39c)}\\
&+ \sum_{f_\alpha\in\mathcal{F}_\alpha\cap\,\partial\Omega} \sum_{t_\beta\in\mathcal{T}_\beta} \left(\frac{\rho(t_\beta)}{\rho_0} - 1\right) \hat{n}^m_{f_\alpha,t_\alpha} \\
&\qquad \int_{f_\alpha} \mathrm{d}^2 r_1 \int_{t_\beta} \mathrm{d}^3 r_2\, \phi_{\mathbf{v}_\alpha,f_\alpha}(\mathbf{r}_1)\, \phi_{\mathbf{v}_\beta,t_\beta}(\mathbf{r}_1)\, \big(\partial^n_1\, g(\mathbf{r}_1-\mathbf{r}_2)\big) && \text{(6.39d)}\\
&- \frac{2}{k^2} \sum_{t_\alpha\in\mathcal{T}_\alpha} \sum_{t_\beta\in\mathcal{T}_\beta} \frac{\mu(t_\beta)}{\lambda_0}\, \frac{1}{h_{\mathbf{v}_\alpha,t_\alpha}}\, \frac{1}{h_{\mathbf{v}_\beta,t_\alpha}}\, \hat{n}^m_{\mathbf{v}_\alpha,t_\alpha}\, \hat{n}^k_{\mathbf{v}_\beta,t_\beta} \\
&\qquad \int_{t_\alpha} \mathrm{d}^3 r_1 \int_{t_\beta} \mathrm{d}^3 r_2\, \big(\partial^k_1\, \partial^n_1\, g(\mathbf{r}_1-\mathbf{r}_2)\big) && \text{(6.39e)}\\
&- \frac{2}{k^2} \sum_{f_\alpha\in\mathcal{F}_\alpha\cap\,\partial\Omega} \sum_{t_\beta\in\mathcal{T}_\beta} \frac{\mu(t_\beta)}{\lambda_0}\, \frac{1}{h_{\mathbf{v}_\beta,t_\alpha}}\, \hat{n}^m_{f_\alpha,t_\alpha}\, \hat{n}^k_{\mathbf{v}_\beta,t_\beta} \\
&\qquad \int_{f_\alpha} \mathrm{d}^2 r_1 \int_{t_\beta} \mathrm{d}^3 r_2\, \phi_{\mathbf{v}_\alpha,f_\alpha}(\mathbf{r}_1)\, \big(\partial^k_1\, \partial^n_1\, g(\mathbf{r}_1-\mathbf{r}_2)\big)\ , && \text{(6.39f)}
\end{aligned}
$$

where v_α is the volume of the tetrahedron t_α. The last two terms, Eqs. (6.39e) and (6.39f), can be integrated by parts and rewritten in a form involving only first derivatives of the Green function, e.g.,

$$
\begin{aligned}
&\int \mathrm{d}^D r_1 \int_{t_\beta} \mathrm{d}^3 r_2\, \cdots\, \big(\partial^k_1\, \partial^n_1\, g(\mathbf{r}_1-\mathbf{r}_2)\big) \\
&= \sum_{f_\beta\in\partial t_\beta} \hat{n}^n_{f_\beta,t_\beta} \int \mathrm{d}^D r_1 \int_{f_\beta} \mathrm{d}^2 r_2\, \cdots\, \big(\partial^k_1\, g(\mathbf{r}_1-\mathbf{r}_2)\big)\ .
\end{aligned}
\tag{6.40}
$$

After substituting this identity in Eqs. (6.39) we would find that some contributions of the facets f_β cancel: this happens whenever the two tetrahedra t adjacent to the face have the

same Lamé coefficient $\mu(t)$. In other words, the contributions to the $\mathbf{r}_2$-integral come only from the discontinuities of μ. We can obtain the same result by integration-by-parts in Eq.(6.38a), which would pick derivatives of μ, hence delta-function contributions.

Similarly, the displacement-pressure and pressure-displacement matrix elements are

$$\begin{aligned}
A^{\mathrm{vp}}_{\mathbf{v}_\alpha,m;\mathbf{v}_\beta} = \frac{\mathrm{i}\,k}{\lambda_0} \sum_{t_\alpha\in\mathcal{T}_\alpha} \sum_{t_\beta\in\mathcal{T}_\beta} \big(\varphi(t_\beta)-1\big)\, \frac{1}{h_{\mathbf{v}_\alpha,\,t_\alpha}}\, \hat{n}^m_{\mathbf{v}_\alpha,\,t_\alpha} \\
\int_{t_\alpha} \mathrm{d}^3r_1 \int_{t_\beta} \mathrm{d}^3r_2\, \phi_{\mathbf{v}_\beta,\,t_\beta}(\mathbf{r}_2)\, g(\mathbf{r}_1-\mathbf{r}_2) \qquad (6.41a) \\
+ \frac{\mathrm{i}\,k}{\lambda_0} \sum_{f_\alpha\in\mathcal{F}_\alpha\cap\,\partial\Omega} \sum_{t_\beta\in\mathcal{T}_\beta} \big(\varphi(t_\beta)-1\big)\, \hat{n}^m_{f_\alpha,\,t_\alpha} \\
\int_{f_\alpha} \mathrm{d}^2r_1 \int_{t_\beta} \mathrm{d}^3r_2\, \phi_{\mathbf{v}_\alpha,\,f_\alpha}(\mathbf{r}_1)\, \phi_{\mathbf{v}_\beta,\,t_\beta}(\mathbf{r}_2)\, g(\mathbf{r}_1-\mathbf{r}_2)\ , \qquad (6.41b)
\end{aligned}$$

and

$$\begin{aligned}
A^{\mathrm{pv}}_{\mathbf{v}_\alpha;\mathbf{v}_\beta,n} = -\,\frac{4\mathrm{i}}{3k} \sum_{t_\alpha\in\mathcal{T}_\alpha} \mu(t_\alpha)\, \frac{1}{h_{\mathbf{v}_\beta,\,t_\alpha}}\, \hat{n}^n_{\mathbf{v}_\beta,\,t_\alpha} \int_{t_\alpha} \mathrm{d}^3r\, \phi_{\mathbf{v}_\alpha,\,t_\alpha}(\mathbf{r}) \qquad (6.42a) \\
-\,\frac{2\mathrm{i}}{3k} \sum_{t_\alpha\in\mathcal{T}_\alpha} \sum_{t_\beta\in\mathcal{T}_\beta} \mu(t_\beta)\, \frac{1}{h_{\mathbf{v}_\beta,\,t_\beta}}\, \hat{n}^k_{\mathbf{v}_\beta,\,t_\beta} \\
\int_{t_\alpha} \mathrm{d}^3r_1 \int_{t_\beta} \mathrm{d}^3r_2\, \phi_{\mathbf{v}_\alpha,\,t_\alpha}(\mathbf{r}_1)\, \big(\partial^k_1\, \partial^n_1\, g(\mathbf{r}_1-\mathbf{r}_2)\big)\ . \qquad (6.42b)
\end{aligned}$$

The second derivatives of the Green function can be eliminated, as in Eqs. (6.39e) and (6.39f), by using the identity (6.40).

Finally, the pressure-pressure matrix elements are given by

$$\begin{aligned}
A^{\mathrm{pp}}_{\mathbf{v}_\alpha;\mathbf{v}_\beta} = -\,k^2 \sum_{t_\alpha\in\mathcal{T}_\alpha} \sum_{t_\beta\in\mathcal{T}_\beta} \big(\varphi(t_\beta)-1\big) \\
\int_{t_\alpha} \mathrm{d}^3r_1 \int_{t_\beta} \mathrm{d}^3r_2\, \phi_{\mathbf{v}_\alpha,\,t_\alpha}(\mathbf{r}_1)\, \phi_{\mathbf{v}_\beta,\,t_\beta}(\mathbf{r}_2)\, g(\mathbf{r}_1-\mathbf{r}_2)\ .
\end{aligned} \qquad (6.43)$$

6.2.4 Summary of the expressions for the "basic" matrix elements

The basic matrix elements appearing in Eqs. (6.39) – (6.43) are as follows:

tetrahedron-tetrahedron matrix elements:

constant-linear:

TT1 $A(t_\alpha;\mathbf{v}_\beta,\,t_\beta) = \int_{t_\alpha} \mathrm{d}^3r_1 \int_{t_\beta} \mathrm{d}^3r_2\, \phi_{\mathbf{v}_\beta,\,t_\beta}(\mathbf{r}_2)\, g(\mathbf{r}_1-\mathbf{r}_2)$

TT2 $A^i(t_\alpha;\mathbf{v}_\beta,\,t_\beta) = \int_{t_\alpha} \mathrm{d}^3r_1 \int_{t_\beta} \mathrm{d}^3r_2\, \phi_{\mathbf{v}_\beta,\,t_\beta}(\mathbf{r}_2)\, \partial^i\, g(\mathbf{r}_1-\mathbf{r}_2)$

linear-linear:

$$\text{TT3}\;\; A(\mathbf{v}_\alpha,\, t_\alpha; \mathbf{v}_\beta,\, t_\beta) = \int_{t_\alpha} \mathrm{d}^3 r_1 \int_{t_\beta} \mathrm{d}^3 r_2\, \phi_{\mathbf{v}_\alpha,\, t_\alpha}(\mathbf{r}_1)\, \phi_{\mathbf{v}_\beta,\, t_\beta}(\mathbf{r}_2)\, g(\mathbf{r}_1 - \mathbf{r}_2)$$

tetrahedron-facet matrix elements:

constant-constant:

$$\text{TF1}\;\; A^i(t_\alpha; f_\beta) = \int_{t_\alpha} \mathrm{d}^3 r_1 \int_{f_\beta} \mathrm{d}^2 r_2\, \partial^i\, g(\mathbf{r}_1 - \mathbf{r}_2)$$

linear-constant:

$$\text{TF2}\;\; A^i(\mathbf{v}_\alpha, t_\alpha; f_\beta) = \int_{t_\alpha} \mathrm{d}^3 r_1 \int_{f_\beta} \mathrm{d}^2 r_2\, \phi_{\mathbf{v}_\alpha,\, t_\alpha}(\mathbf{r}_1)\, \partial^i\, g(\mathbf{r}_1 - \mathbf{r}_2)$$

linear-linear:

$$\text{TF3}\;\; A(\mathbf{v}_\alpha,\, t_\alpha; \mathbf{v}_\beta,\, f_\beta) = \int_{t_\alpha} \mathrm{d}^3 r_1 \int_{f_\beta} \mathrm{d}^2 r_2\, \phi_{\mathbf{v}_\alpha,\, t_\alpha}(\mathbf{r}_1)\, \phi_{\mathbf{v}_\beta,\, f_\beta}(\mathbf{r}_2)\, g(\mathbf{r}_1 - \mathbf{r}_2)$$

$$\text{TF4}\;\; A^i(\mathbf{v}_\alpha,\, t_\alpha; \mathbf{v}_\beta,\, f_\beta) = \int_{t_\alpha} \mathrm{d}^3 r_1 \int_{f_\beta} \mathrm{d}^2 r_2\, \phi_{\mathbf{v}_\alpha,\, t_\alpha}(\mathbf{r}_1)\, \phi_{\mathbf{v}_\beta,\, f_\beta}(\mathbf{r}_2)\, \partial^i\, g(\mathbf{r}_1 - \mathbf{r}_2)$$

facet-facet matrix elements:

linear-constant:

$$\text{FF1}\;\; A^i(\mathbf{v}_\alpha, f_\alpha; f_\beta) = \int_{f_\alpha} \mathrm{d}^2 r_1 \int_{f_\beta} \mathrm{d}^2 r_2\, \phi_{\mathbf{v}_\alpha,\, t_\alpha}(\mathbf{r}_1)\, \partial^i\, g(\mathbf{r}_1 - \mathbf{r}_2)$$

Whenever derivatives of the Green function appear, they are not normal derivatives.

6.3 Integral equations in second-order formulation

Eqs. (3.9) have the general form of an "L-S-type" differential equation with three alternative expressions for the differential operator $\mathcal{V}$. It can be easily verified that the background-medium Green function $g = -\mathcal{D}^{-1}$ is given by

$$g_{ij}(\mathbf{r}) = -k^{-2}\, \left[\delta_{ij}\, \delta^3(\mathbf{r}) + \partial_i\, \partial_j\, g(\mathbf{r})\right]\;, \tag{6.44}$$

and satisfies the equation

$$(k^2\, \delta_{ij} + \partial_i\, \partial_j)\, g_{jl}(\mathbf{r}) = -\,\delta_{il}\, \delta^3(\mathbf{r}) \tag{6.45}$$

and the outgoing-wave boundary conditions. The resulting L-S equation

$$u_i(\mathbf{r}) - \int \mathrm{d}^3 r'\, g_{il}(\mathbf{r} - \mathbf{r}')\, \mathcal{V}_{lj}(\mathbf{r}')\, u_j(\mathbf{r}') = u_i^{\mathrm{in}}(\mathbf{r}') \tag{6.46}$$

becomes then, with Eq.(6.44),

$$u_i(\mathbf{r}) + k^{-2}\,\mathcal{V}_{ij}(\mathbf{r})\,u_j(\mathbf{r}') + k^{-2}\int \mathrm{d}^3r'\,\partial_i\,\partial_l\,g(\mathbf{r}-\mathbf{r}')\,\mathcal{V}_{lj}(\mathbf{r}')\,u_j(\mathbf{r}') = u_i^{\mathrm{in}}(\mathbf{r}')\ . \tag{6.47}$$

Depending on the form of the differential equation, various forms of the L-S equations can be obtained. In the following we consider three such forms, corresponding to Eqs. (3.9a), (3.9b), and (3.9c), and we refer to them as equations of type (a), (b), and (c).

The interaction operator $\mathcal{V}$ derived from the differential equation (3.9a) gives rise to an L-S equation of the "basic" form

$$\begin{aligned}
&u_i(\mathbf{r}) - \left(1-\frac{\rho(\mathbf{r})}{\rho_0}\right)u_i(\mathbf{r}) - k^2\,\partial_i\left[\left(1-\frac{\lambda(\mathbf{r})}{\lambda_0}\right)\partial_j u_j(\mathbf{r})\right] + k^2\,\partial_j\left[\frac{\mu(\mathbf{r})}{\lambda_0}\,\Big(\partial_i u_j(\mathbf{r}) + \partial_j u_i(\mathbf{r})\Big)\right] \\
&\quad - \int \mathrm{d}^3r'\,\partial_i\,\partial_l\,g(\mathbf{r}-\mathbf{r}')\left(1-\frac{\rho(\mathbf{r}')}{\rho_0}\right)u_l(\mathbf{r}') \\
&\quad - k^{-2}\int \mathrm{d}^3r'\,\partial_i\,\partial_l\,g(\mathbf{r}-\mathbf{r}')\,\partial'_l\left[\left(1-\frac{\lambda(\mathbf{r}')}{\lambda_0}\right)\partial'_j u_j(\mathbf{r}')\right] \\
&\quad + k^{-2}\int \mathrm{d}^3r'\,\partial_i\,\partial_l\,g(\mathbf{r}-\mathbf{r}')\,\partial'_j\left[\frac{\mu(\mathbf{r}')}{\lambda_0}\,\Big(\partial'_l u_j(\mathbf{r}') + \partial'_j u_l(\mathbf{r}')\Big)\right] \\
&\quad = u_i^{\mathrm{in}}(\mathbf{r})\ .
\end{aligned} \tag{6.48}$$

With the operator $\mathcal{V}$ corresponding to Eq.(3.9b) we obtain

$$\begin{aligned}
&u_i(\mathbf{r}) + k^{-2}\,\frac{\rho_0}{\rho(\mathbf{r})}\,\partial_j\left[\frac{\mu(\mathbf{r})}{\lambda_0}\,\Big(\partial_i u_j(\mathbf{r}) + \partial_j u_i(\mathbf{r})\Big)\right] - k^{-2}\left(\partial_i\,\frac{\rho_0}{\rho(\mathbf{r})}\right)\frac{\lambda(\mathbf{r})}{\lambda_0}\,\partial_j u_j(\mathbf{r}) \\
&\quad + \int \mathrm{d}^3r'\,\partial_i\,g(\mathbf{r}-\mathbf{r}')\left[1-\frac{\rho_0\,\lambda(\mathbf{r}')}{\lambda_0\,\rho(\mathbf{r}')}\right]\partial'_j\,u_j(\mathbf{r}') \\
&\quad + k^{-2}\int \mathrm{d}^3r'\,\partial_i\,\partial_l\,g(\mathbf{r}-\mathbf{r}')\,\frac{\rho_0}{\rho(\mathbf{r}')}\,\partial'_j\left[\frac{\mu(\mathbf{r}')}{\lambda_0}\,\Big(\partial'_l\,u_j(\mathbf{r}') + \partial'_j\,u_l(\mathbf{r}')\Big)\right] \\
&\quad - k^{-2}\int \mathrm{d}^3r'\,\partial_i\,\partial_l\,g(\mathbf{r}-\mathbf{r}')\left(\partial'_l\,\frac{\rho_0}{\rho(\mathbf{r}')}\right)\frac{\lambda(\mathbf{r}')}{\lambda_0}\,\partial'_j\,u_j(\mathbf{r}') \\
&\quad = u_i^{\mathrm{in}}(\mathbf{r})\ ,
\end{aligned} \tag{6.49}$$

where ∂ and ∂' denote derivatives with respect to $\mathbf{r}$ and $\mathbf{r}'$.

In deriving Eq.(6.49) we applied integration by parts to the term

$$-k^{-2}\int \mathrm{d}^3r'\,\partial_i\,\partial_l\,g(\mathbf{r}-\mathbf{r}')\ \partial'_l\ \left\{\left[1-\frac{\rho_0\,\lambda(\mathbf{r}')}{\lambda_0\,\rho(\mathbf{r}')}\right]\ \partial'_j\,u_j(\mathbf{r}')\right\}\ ,$$

resulting from directly from the original L-S equation of (6.47). We apply here the derivative ∂_l to the Green function, and use its defining equation to obtain the fourth term in Eq.(6.49) with a single derivative of the Green function.

The boundary term in integration by parts vanishes because the material-dependent term (in the square brackets) vanishes outside $\overline{\Omega}$.

Finally, with the operator $\mathcal{V}$ of Eq.(3.9c) the L-S equation takes the form

$$
\begin{aligned}
& u_i(\mathbf{r}) && \text{(6.50a)}\\
& + k^{-2}\,\partial_j \left[\xi_\mu(\mathbf{r}) \left(\partial_i u_j(\mathbf{r}) + \partial_j u_i(\mathbf{r})\right)\right] && \text{(6.50b)}\\
& - k^{-2} \left(\partial_j \frac{\rho_0}{\rho(\mathbf{r})}\right) \frac{\rho(\mathbf{r})}{\rho_0} \\
& \qquad \left[\xi_\lambda(\mathbf{r})\ \delta_{ij}\ \partial_k u_k(\mathbf{r}) + \xi_\mu(\mathbf{r}) \left(\partial_i u_j(\mathbf{r}) + \partial_j u_i(\mathbf{r})\right)\right] && \text{(6.50c)}\\
& + \int \mathrm{d}^3 r'\, \partial_i\, g(\mathbf{r}-\mathbf{r}')\, [1-\xi_\lambda(\mathbf{r}')]\, \partial'_k u_k(\mathbf{r}') && \text{(6.50d)}\\
& + k^{-2} \int \mathrm{d}^3 r'\, \partial_i\, \partial_l\, g(\mathbf{r}-\mathbf{r}')\, \partial'_j \left[\xi_\mu(\mathbf{r}') \left(\partial'_l u_j(\mathbf{r}') + \partial'_j u_l(\mathbf{r}')\right)\right] && \text{(6.50e)}\\
& - k^{-2} \int \mathrm{d}^3 r'\, \partial_i\, \partial_l\, g(\mathbf{r}-\mathbf{r}') \left(\partial'_j \frac{\rho_0}{\rho(\mathbf{r}')}\right) \\
& \qquad \left[\eta_\lambda(\mathbf{r}')\ \delta_{lj}\ \partial'_k u_k(\mathbf{r}') + \eta_\mu(\mathbf{r}') \left(\partial'_l u_j(\mathbf{r}') + \partial'_j u_l(\mathbf{r}')\right)\right] && \text{(6.50f)}\\
& = u_i^{\mathrm{in}}(\mathbf{r})\ , && \text{(6.50g)}
\end{aligned}
$$

or, after some rearrangements and integration by parts,

$$
\begin{aligned}
& u_i(\mathbf{r}) && \mathcal{O}(1) \quad \text{(6.51a)}\\
& - k^{-2}\,\partial_j \left[\left(1-\xi_\lambda(\mathbf{r})\right) \delta_{ij} \partial_k u_k(\mathbf{r}) - \xi_\mu(\mathbf{r}) \left(\partial_i u_j(\mathbf{r}) + \partial_j u_i(\mathbf{r})\right)\right] && \mathcal{O}(\rho_0/\rho) \quad \text{(6.51b)}\\
& - k^{-2} \left(\partial_j \frac{\rho_0}{\rho(\mathbf{r})}\right) \\
& \qquad \left[\eta_\lambda(\mathbf{r})\ \delta_{ij}\ \partial_k u_k(\mathbf{r}) + \eta_\mu(\mathbf{r}) \left(\partial_i u_j(\mathbf{r}) + \partial_j u_i(\mathbf{r})\right)\right] && \mathcal{O}(1) \quad \text{(6.51c)}\\
& - k^{-2} \int \mathrm{d}^3 r'\, \partial_i\, \partial_l\, \partial_j\, g(\mathbf{r}-\mathbf{r}') \\
& \qquad \left[\left(1-\xi_\lambda(\mathbf{r}')\right)\ \delta_{lj}\ \partial'_k u_k(\mathbf{r}') - \xi_\mu(\mathbf{r}') \left(\partial'_l u_j(\mathbf{r}') + \partial'_j u_l(\mathbf{r}')\right)\right] && \mathcal{O}(\rho_0/\rho) \quad \text{(6.51d)}\\
& - k^{-2} \int \mathrm{d}^3 r'\, \partial_i\, \partial_l\, g(\mathbf{r}-\mathbf{r}') \left(\partial'_j \frac{\rho_0}{\rho(\mathbf{r}')}\right) \\
& \qquad \left[\eta_\lambda(\mathbf{r}')\ \delta_{lj}\ \partial'_k u_k(\mathbf{r}') + \eta_\mu(\mathbf{r}') \left(\partial'_l u_j(\mathbf{r}') + \partial'_j u_l(\mathbf{r}')\right)\right] && \mathcal{O}(1) \quad \text{(6.51e)}\\
& = u_i^{\mathrm{in}}(\mathbf{r})\ . && \mathcal{O}(1) \quad \text{(6.51f)}
\end{aligned}
$$

In the last forms of the L-S equation we indicated, next to each term, its expected magnitude in the high contrast limit $\rho_0/\rho \to 0$ (the origin of these estimates is discussed below).

There are two reasons we consider Eq.(6.51) our preferred form of the L-S integral equation:

(i) As shown by the estimates above, only two nontrivial terms in the equation, (6.51c) and (6.51e), remain sizable in the high contrast limit. Both of these terms involve the gradient of the inverse of density, and, therefore, give rise to surface contribution from interfaces of regions of large density ratios.

(ii) The term (6.51e) involves an expression proportional to the ***stress tensor*** σ,

$$\eta_\lambda \, \delta_{ij} \, \partial_l u_l + \eta_\mu \, \left(\partial_i u_j + \partial_j u_i\right) \equiv \frac{1}{\lambda_0} \, \sigma_{ij} \; . \tag{6.52}$$

Contraction of this quantity with the gradient of the inverse density, i.e., with the normal to the surface of density discontinuity, is proportional the ***traction vector***, which is known to be ***continuous*** across that surface. The latter property facilitates discretization of the equations in the case of a discontinuous density distribution, since the product of the gradient of the density ratio (a surface delta function) and a continuous function is unambiguously defined.

The estimates of the magnitudes of the terms in Eq.(6.51) follow from an important scaling property of Eqs. (3.9c) and (6.51): while the coefficients involving gradients of ρ_0/ρ grow proportionally to ρ/ρ_0, their product with the solution remains finite, since the stress tensor (6.52) is finite in the high density limit, and thus the gradients of the displacement in Eq.(6.51) are ***small***:

$$\partial_i \, u_j \sim \frac{\rho_0}{\rho} \tag{6.53}$$

(we recall that Eq.(3.10) implies $\xi_\lambda \sim \xi_\mu \sim 1$ for finite values of refraction coefficients). This is the reason why, in Eq.(6.51), the terms *without* derivatives of the density and factors ρ/ρ_0, are small. In particular, the fifth term (6.51e) in the equation, involving the gradient of ξ_μ (and thus possibly a surface delta function due to a discontinuity in μ) is small compared to the dominant terms, (6.51c) and (6.51e).

6.3.1 Matrix elements for the “basic” form of second-order equations: general expressions

The most basic form of the L-S equation, (6.48), gives rise to the nontrivial Galerkin matrix elements[1]

$$A^{(\rho)}_{\alpha\beta} = -\int \mathrm{d}^3 r_1 \int \mathrm{d}^3 r_2 \, \psi^i_\alpha(\mathbf{r}_1) \left(\partial^i_1 \, \partial^l_1 \, g(\mathbf{r}_1 - \mathbf{r}_2)\right) \left(1 - \rho(\mathbf{r}_2)\right) \psi^l_\beta(\mathbf{r}_2)\big) \; , \tag{6.54a}$$

$$\begin{aligned} A^{(\lambda)}_{\alpha\beta} = & - k^{-2} \int \mathrm{d}^3 r_1 \int \mathrm{d}^3 r_2 \, \psi^i_\alpha(\mathbf{r}_1) \left(\partial^i_1 \, \partial^l_1 \, g(\mathbf{r}_1 - \mathbf{r}_2)\right) \\ & \qquad \partial^l_2 \left[\left(1 - \lambda(\mathbf{r}_2)\right) \partial^j_2 \, \psi^j_\beta(\mathbf{r}_2)\right] \; , \end{aligned} \tag{6.54b}$$

$$\begin{aligned} A^{(\mu)}_{\alpha\beta} = & \; k^{-2} \int \mathrm{d}^3 r_1 \int \mathrm{d}^3 r_2 \, \psi^i_\alpha(\mathbf{r}_1) \left(\partial^i_1 \, \partial^l_1 \, g(\mathbf{r}_1 - \mathbf{r}_2)\right) \\ & \qquad \partial^j_2 \left[\mu(\mathbf{r}_2) \left(\partial^l_2 \, \psi^j_\beta(\mathbf{r}_2) + \partial^j_2 \, \psi^l_\beta(\mathbf{r}_2)\right)\right] \end{aligned} \tag{6.54c}$$

[1]In order to simplify the notation, we assume here, temporarily, $\rho_0 = \lambda_0 = 1$.

(the other matrix elements involve single integrals only). After integrating by parts with respect to $\mathbf{r}_1$, we find, alternatively

$$A_{\alpha\beta}^{(\rho)} = \int \mathrm{d}^3 r_1 \int \mathrm{d}^3 r_2 \left(\partial_1^i \, \psi_\alpha^i(\mathbf{r}_1)\right) \left(\partial_1^l \, g(\mathbf{r}_1 - \mathbf{r}_2)\right) \left(1 - \rho(\mathbf{r}_2)\right) \psi_\beta^l(\mathbf{r}_2)\right) , \tag{6.55a}$$

$$A_{\alpha\beta}^{(\lambda)} = k^{-2} \int \mathrm{d}^3 r_1 \int \mathrm{d}^3 r_2 \left(\partial_1^i \, \psi_\alpha^i(\mathbf{r}_1)\right) \left(\partial_1^l \, g(\mathbf{r}_1 - \mathbf{r}_2)\right) \partial_2^l \left[\left(1 - \lambda(\mathbf{r}_2)\right) \partial_2^j \, \psi_\beta^j(\mathbf{r}_2)\right] , \tag{6.55b}$$

$$A_{\alpha\beta}^{(\mu)} = - \, k^{-2} \int \mathrm{d}^3 r_1 \int \mathrm{d}^3 r_2 \left(\partial_1^i \, \psi_\alpha^i(\mathbf{r}_1)\right) \left(\partial_1^l \, g(\mathbf{r}_1 - \mathbf{r}_2)\right) \partial_2^j \left[\mu(\mathbf{r}_2) \left(\partial_2^l \, \psi_\beta^j(\mathbf{r}_2) + \partial_2^j \, \psi_\beta^l(\mathbf{r}_2)\right)\right] \tag{6.55c}$$

or

$$A_{\alpha\beta}^{(\rho)} = \int \mathrm{d}^3 r_1 \int \mathrm{d}^3 r_2 \left(\partial_1^l \, \psi_\alpha^i(\mathbf{r}_1)\right) \left(\partial_1^i \, g(\mathbf{r}_1 - \mathbf{r}_2)\right) \left(1 - \rho(\mathbf{r}_2)\right) \psi_\beta^l(\mathbf{r}_2)\right) , \tag{6.56a}$$

$$A_{\alpha\beta}^{(\lambda)} = k^{-2} \int \mathrm{d}^3 r_1 \int \mathrm{d}^3 r_2 \left(\partial_1^l \, \psi_\alpha^i(\mathbf{r}_1)\right) \left(\partial_1^i \, g(\mathbf{r}_1 - \mathbf{r}_2)\right) \partial_2^l \left[\left(1 - \lambda(\mathbf{r}_2)\right) \partial_2^j \, \psi_\beta^j(\mathbf{r}_2)\right] , \tag{6.56b}$$

$$A_{\alpha\beta}^{(\mu)} = - \, k^{-2} \int \mathrm{d}^3 r_1 \int \mathrm{d}^3 r_2 \left(\partial_1^l \, \psi_\alpha^i(\mathbf{r}_1)\right) \left(\partial_1^i \, g(\mathbf{r}_1 - \mathbf{r}_2)\right) \partial_2^j \left[\mu(\mathbf{r}_2) \left(\partial_2^l \, \psi_\beta^j(\mathbf{r}_2) + \partial_2^j \, \psi_\beta^l(\mathbf{r}_2)\right)\right] \tag{6.56c}$$

Expected features of the matrix elements. We note that in Eqs. (6.55) the basis function ψ_α appears only in its divergence. For linear basis functions (Section 6.1.1), this divergence involves constant basis functions supported on tetrahedra and delta functions supported on facets located on the boundary $\partial\Omega$ of the object, since (as discussed following Eq.(6.3)) the other delta-function contributions cancel pairwise, due to continuity of the basis function.

Eqs. (6.56) involve, instead of the divergence of ψ_α, a general element of the strain tensor associated with this basis functions. However, the regularity structure of this expression is similar to the previous one.

On the other hand, derivatives of the basis function ψ_β do, in general, include delta-function contributions from facets shared by tetrahedra supporting the basis function (since material parameters may have different values on different tetrahedra).

Further, Eqs. (6.55b) and (6.55c), as well as Eqs. (6.56b) and (6.56c), include, in general, delta functions due to discontinuities of the material parameters on facets. In Eqs. (6.56b) and (6.56c) the product of these delta functions and the derivatives of the basis function should be well defined, for reasons analogous to those in acoustics: We note that the sum of the matrix elements (6.55b) and (6.55c) the considered delta functions appear only through

the expression

$$
\begin{aligned}
&-\int \mathrm{d}^3 r_2 \left(\partial_1^l\, g(\mathbf{r}_1-\mathbf{r}_2)\right) \\
&\qquad\qquad \left[\left(\partial_2^l\, \lambda(\mathbf{r}_2)\right) \partial_2^j\, \psi_\beta^j(\mathbf{r}_2) + \left(\partial_2^j\, \mu(\mathbf{r}_2)\right) \left(\partial_2^l\, \psi_\beta^j(\mathbf{r}_2) + \partial_2^j\, \psi_\beta^l(\mathbf{r}_2)\right)\right] \\
=& -\int_{f_2} \mathrm{d}^2 r_2 \left(\partial_1^l\, g(\mathbf{r}_1-\mathbf{r}_2)\right) \\
&\qquad\qquad \hat{n}_2^j \left[\left(\lambda(t_2+) - \lambda(t_2-)\right) \delta_{lj}\, \partial_2^p\, \psi_\beta^p(\mathbf{r}_2)\right. \\
&\qquad\qquad\quad \left. + \left(\mu(t_2+) - \mu(t_2-)\right) \left(\partial_2^l\, \psi_\beta^j(\mathbf{r}_2) + \partial_2^j\, \psi_\beta^l(\mathbf{r}_2)\right)\right] \\
=& -\int_{f_2} \mathrm{d}^2 r_2 \left(\partial_1^l\, g(\mathbf{r}_1-\mathbf{r}_2)\right) \hat{n}_2^j \\
&\qquad\qquad \Big\{\left[\lambda(t_2+)\, \delta_{lj}\, \partial_2^p\, \psi_\beta^p(\mathbf{r}_2) + \mu(t_2+) \left(\partial_2^l\, \psi_\beta^j(\mathbf{r}_2) + \partial_2^j\, \psi_\beta^l(\mathbf{r}_2)\right)\right] \\
&\qquad\qquad - \left[(t_2+ \to t_2-)\right]\Big\} \\
\equiv& -\int_{f_2} \mathrm{d}^2 r_2 \left(\partial_1^l\, g(\mathbf{r}_1-\mathbf{r}_2)\right) \hat{n}_2^j \left\{\sigma_{lj}(t_2+) - \sigma_{lj}(t_2-)\right\} \, .
\end{aligned}
\tag{6.57}
$$

6.3.2 Matrix elements for the "high-contrast" form of second-order equations: general expressions

We denote in the following by the subscripts (a) to (f) the contributions to the matrix elements corresponding to terms in Eqs. (6.51a) to (6.51e):

$$A^{(a)}_{\alpha\beta} = \int \mathrm{d}^3r\, \psi^i_\alpha(\mathbf{r})\, \psi^i_\beta(\mathbf{r}) \ , \tag{6.58a}$$

$$A^{(b)}_{\alpha\beta} = k^{-2} \int \mathrm{d}^3r \left(\partial^i\, \psi^j_\alpha(\mathbf{r})\right) \left[\left(1 - \xi_\lambda(\mathbf{r})\right) \delta_{ij}\, \partial^k \psi^k_\beta(\mathbf{r}) - \xi_\mu(\mathbf{r}) \left(\partial^i\, \psi^j_\beta(\mathbf{r}) + \partial^j\, \psi^i_\beta(\mathbf{r})\right)\right] \ , \tag{6.58b}$$

$$A^{(c)}_{\alpha\beta} = -\, k^2 \int \mathrm{d}^3r\, \psi^i_\alpha(\mathbf{r}) \left(\partial^j\, \frac{\rho_0}{\rho(\mathbf{r})}\right) \frac{\rho(\mathbf{r})}{\rho_0} \left[\xi_\lambda(\mathbf{r})\ \delta_{ij}\, \partial^k \psi^k_\beta(\mathbf{r}) + \xi_\mu(\mathbf{r}) \left(\partial^i \psi^j_\beta(\mathbf{r}) + \partial^j \psi^i_\beta(\mathbf{r})\right)\right] \ , \tag{6.58c}$$

$$\begin{aligned} A^{(d)}_{\alpha\beta} &= -\, k^{-2} \int \mathrm{d}^3r_1 \int \mathrm{d}^3r_2 \left(\partial^i_1\, \partial^l_1\, \psi^l_\alpha(\mathbf{r}_1)\right) g(\mathbf{r}_1 - \mathbf{r}_2) \\ &\qquad \partial^j_2 \left[\left(1 - \xi_\lambda(\mathbf{r}_2)\right) \delta_{ij}\, \partial^k_2 \psi^k_\beta(\mathbf{r}_2) - \xi_\mu(\mathbf{r}_2) \left(\partial^i_2\, \psi^j_\beta(\mathbf{r}_2) + \partial^j_2\, \psi^i_\beta(\mathbf{r}_2)\right)\right] \\ &\equiv k^{-2} \int \mathrm{d}^3r_1 \int \mathrm{d}^3r_2 \left(\partial^l_1\, \psi^l_\alpha(\mathbf{r}_1)\right) \left(\partial^i_1\, g(\mathbf{r}_1 - \mathbf{r}_2)\right) \\ &\qquad \partial^j_2 \left[\left(1 - \xi_\lambda(\mathbf{r}_2)\right) \delta_{ij}\, \partial^k_2 \psi^k_\beta(\mathbf{r}_2) - \xi_\mu(\mathbf{r}_2) \left(\partial^i_2\, \psi^j_\beta(\mathbf{r}_2) + \partial^j_2\, \psi^i_\beta(\mathbf{r}_2)\right)\right] \ , \end{aligned} \tag{6.58d}$$

$$\begin{aligned} A^{(e)}_{\alpha\beta} &= -\, k^{-2} \int \mathrm{d}^3r_1 \int \mathrm{d}^3r_2 \left(\partial^i_1\, \partial^l_1\, \psi^l_\alpha(\mathbf{r}_1)\right) g(\mathbf{r}_1 - \mathbf{r}_2) \left(\partial^j_2 \frac{\rho_0}{\rho(\mathbf{r}_2)}\right) \\ &\qquad \left[\eta_\lambda(\mathbf{r}_2)\ \delta_{ij}\, \partial^k_2 \psi^k_\beta(\mathbf{r}_2) + \eta_\mu(\mathbf{r}_2) \left(\partial^i_2 \psi^j_\beta(\mathbf{r}_2) + \partial^j_2 \psi^i_\beta(\mathbf{r}_2)\right)\right] \\ &\equiv k^{-2} \int \mathrm{d}^3r_1 \int \mathrm{d}^3r_2 \left(\partial^l_1\, \psi^l_\alpha(\mathbf{r}_1)\right) \left(\partial^i_1\, g(\mathbf{r}_1 - \mathbf{r}_2)\right) \left(\partial^j_2 \frac{\rho_0}{\rho(\mathbf{r}_2)}\right) \\ &\qquad \left[\eta_\lambda(\mathbf{r}_2)\ \delta_{ij}\, \partial^k_2 \psi^k_\beta(\mathbf{r}_2) + \eta_\mu(\mathbf{r}_2) \left(\partial^i_2 \psi^j_\beta(\mathbf{r}_2) + \partial^j_2 \psi^i_\beta(\mathbf{r}_2)\right)\right] . \end{aligned} \tag{6.58e}$$

6.3.3 Matrix elements with composite linear basis functions

After carrying out the index algebra in Eqs. (6.58), the matrix elements can be represents in terms of the scalar basis functions as follows:

$$A^{(a)}_{\mathbf{v}_\alpha,m;\mathbf{v}_\beta,n} = \delta_{mn} \int \mathrm{d}^3r\, \phi_{\mathbf{v}_\alpha}(\mathbf{r})\, \phi_{\mathbf{v}_\beta}(\mathbf{r}) \ , \tag{6.59a}$$

$$\begin{aligned} A^{(b)}_{\mathbf{v}_\alpha,m;\mathbf{v}_\beta,n} = &-k^{-2} \int \mathrm{d}^3r\, \left(\partial^i \phi_{\mathbf{v}_\alpha}(\mathbf{r})\right) \\ &\left[\xi_\lambda(\mathbf{r})\, \delta_{nl}\, \delta_{im} + \xi_\mu(\mathbf{r})\, \left(\delta_{ni}\, \delta_{lm} + \delta_{nm}\, \delta_{li}\right)\right]\, \left(\partial^l\, \phi_{\mathbf{v}_\beta}(\mathbf{r})\right) \ , \end{aligned} \tag{6.59b}$$

$$\begin{aligned} A^{(c)}_{\mathbf{v}_\alpha,m;\mathbf{v}_\beta,n} = &-k^2 \int \mathrm{d}^3r\, \phi_{\mathbf{v}_\alpha}(\mathbf{r}) \left(\partial^i \frac{\rho_0}{\rho(\mathbf{r})}\right) \frac{\rho(\mathbf{r})}{\rho_0} \\ &\left[\xi_\lambda(\mathbf{r})\, \delta_{nl}\, \delta_{im} + \xi_\mu(\mathbf{r})\, \left(\delta_{ni}\, \delta_{lm} + \delta_{nm}\, \delta_{li}\right)\right]\, \left(\partial^l\, \phi_{\mathbf{v}_\beta}(\mathbf{r})\right) \ , \end{aligned} \tag{6.59c}$$

$$\begin{aligned} A^{(d)}_{\mathbf{v}_\alpha,m;\mathbf{v}_\beta,n} = &\, k^{-2} \int \mathrm{d}^3r_1 \int \mathrm{d}^3r_2\, \left(\partial_1^m\, \phi_{\mathbf{v}_\alpha}(\mathbf{r}_1)\right) \left(\partial_1^i\, g(\mathbf{r}_1 - \mathbf{r}_2)\right) \\ &\partial_2^j \left\{\left[\left(1 - \xi_\lambda(\mathbf{r}_2)\right) \delta_{nl}\, \delta_{ij} - \xi_\mu(\mathbf{r}_2)\, \left(\delta_{ni}\, \delta_{lj} + \delta_{nj}\, \delta_{li}\right)\right]\, \left(\partial_2^l\, \phi_{\mathbf{v}_\beta}(\mathbf{r}_2)\right)\right\} \\ \equiv &-k^{-2} \int \mathrm{d}^3r_1 \int \mathrm{d}^3r_2\, \left(\partial_1^m\, \partial_1^i\, \phi_{\mathbf{v}_\alpha}(\mathbf{r}_1)\right) \left(\partial_1^j\, g(\mathbf{r}_1 - \mathbf{r}_2)\right) \\ &\left[\left(1 - \xi_\lambda(\mathbf{r}_2)\right) \delta_{nl}\, \delta_{ij} - \xi_\mu(\mathbf{r}_2)\, \left(\delta_{ni}\, \delta_{lj} + \delta_{nj}\, \delta_{li}\right)\right]\, \left(\partial_2^l\, \phi_{\mathbf{v}_\beta}(\mathbf{r}_2)\right) \\ \equiv &-k^{-2} \int \mathrm{d}^3r_1 \int \mathrm{d}^3r_2\, \left(\partial_1^m\, \partial_1^i\, \phi_{\mathbf{v}_\alpha}(\mathbf{r}_1)\right) g(\mathbf{r}_1 - \mathbf{r}_2) \\ &\partial_2^j \left\{\left[\left(1 - \xi_\lambda(\mathbf{r}_2)\right) \delta_{nl}\, \delta_{ij} - \xi_\mu(\mathbf{r}_2)\, \left(\delta_{ni}\, \delta_{lj} + \delta_{nj}\, \delta_{li}\right)\right]\, \left(\partial_2^l\, \phi_{\mathbf{v}_\beta}(\mathbf{r}_2)\right)\right\} \ , \end{aligned} \tag{6.59d}$$

$$\begin{aligned} A^{(e)}_{\mathbf{v}_\alpha,m;\mathbf{v}_\beta,n} = &\, k^{-2} \int \mathrm{d}^3r_1 \int \mathrm{d}^3r_2\, \left(\partial_1^m\, \phi_{\mathbf{v}_\alpha}(\mathbf{r}_1)\right) \left(\partial_1^i\, g(\mathbf{r}_1 - \mathbf{r}_2)\right) \left(\partial_2^j \frac{\rho_0}{\rho(\mathbf{r}_2)}\right) \\ &\left[\eta_\lambda(\mathbf{r}_2)\, \delta_{nl}\, \delta_{ij} + \eta_\mu(\mathbf{r}_2)\, \left(\delta_{ni}\, \delta_{lj} + \delta_{nj}\, \delta_{li}\right)\right]\, \left(\partial_2^l\, \phi_{\mathbf{v}_\beta}(\mathbf{r}_2)\right) \\ \equiv &-k^{-2} \int \mathrm{d}^3r_1 \int \mathrm{d}^3r_2\, \left(\partial_1^m\, \partial_1^i\, \phi_{\mathbf{v}_\alpha}(\mathbf{r}_1)\right) g(\mathbf{r}_1 - \mathbf{r}_2) \left(\partial_2^j \frac{\rho_0}{\rho(\mathbf{r}_2)}\right) \\ &\left[\eta_\lambda(\mathbf{r}_2)\, \delta_{nl}\, \delta_{ij} + \eta_\mu(\mathbf{r}_2)\, \left(\delta_{ni}\, \delta_{lj} + \delta_{nj}\, \delta_{li}\right)\right]\, \left(\partial_2^l\, \phi_{\mathbf{v}_\beta}(\mathbf{r}_2)\right) \ . \end{aligned} \tag{6.59e}$$

In the following we specialize to the case of material parameters constant on tetrahedra, and to piecewise linear basis functions $\phi_{\mathbf{v}}(\mathbf{r})$. The matrix elements Eq.(6.59) exhibit then analogies to the acoustic problem with piecewise linear basis functions, since a derivative of a linear basis function is a constant – plus, possibly, a delta-function at the boundary of the tetrahedron. The main difficulty lies in treating the possible delta-function contributions.

Eqs. (6.59d) and (6.59e) appear in several equivalent forms related by integration by parts: they differ in the numbers of derivatives acting on the Green function and on the basis functions $\boldsymbol{\psi}_\alpha$ or $\boldsymbol{\psi}_\beta$ (Eq.(6.9)). The forms with fewer derivatives acting on on the Green function are more appropriate for computing matrix elements at small distances (for overlapping basis functions' supports), and the other forms are more useful for larger distances, where the derivatives of the Green function reflects the large-distance behavior of the matrix elements.

6.3.4 Matrix elements with elementary linear basis functions

Eqs. (6.59) involve "composite" linear scalar basis functions associated with vertices, i.e., supported on sets of tetrahedra. In the following we use the relations of Section 6.1.1 to express these functions in terms of "elementary" basis functions supported on individual tetrahedra or facets (the latter arise as a result of differentiation of the volumetric basis functions).

We give below explicit expression for the individual contributions to the matrix elements. We will generally concentrate on the expressions with the largest numbers of derivatives of the basis functions, since such terms may contain surface contributions.

The term $A^{(a)}$: In this simplest case we obtain a sum of contributions of tetrahedra t shared by the vertices $\mathbf{v}_\alpha$ and $\mathbf{v}_\beta$, i.e., belonging to the set $\mathcal{T}_\alpha \cap \mathcal{T}_\beta$. Each term is an analytic expression for the integral of a product of two linear functions supported on the tetrahedron t.

The terms $A^{(b)}$ and $A^{(c)}$: The term $A^{(b)}$ involves derivatives of the basis function $\boldsymbol{\psi}_{\mathbf{v}_\alpha,m}$ which, according to Eqs. (6.1) and (6.3), can be expressed in terms of basis functions supported on tetrahedra as

$$\partial^i \phi_{\mathbf{v}_\alpha}(\mathbf{r}) = -\sum_{t_\alpha \in \mathcal{T}_\alpha} \left[\frac{1}{h_{\mathbf{v}_\alpha, t_\alpha}} \hat{n}^i_{\mathbf{v}_\alpha, t_\alpha} \, \chi_{t_\alpha}(\mathbf{r}) + \sum_{f_\alpha \in \partial t_\alpha} \phi_{\mathbf{v}_\alpha, f_\alpha}(\mathbf{r}) \, \hat{n}^i_{f_\alpha, t_\alpha} \, \delta_{f_\alpha}(\mathbf{r}) \right] , \tag{6.60}$$

where, we recall, $h_{\mathbf{v}_\alpha, t_\alpha}$ the height of the tetrahedron t_α measured from the vertex $\mathbf{v}_\alpha$, $\hat{\mathbf{n}}_{\mathbf{v}_\alpha, t_\alpha}$ is the exterior unit normal to the tetrahedron facet opposite the same vertex, and $\hat{\mathbf{n}}_{f_\alpha, t_\alpha}$ is the unit normal to the face f_α, in the direction exterior to the tetrahedron t_α.

The outer sum in Eq.(6.60) runs over tetrahedra $t_\alpha \in \mathcal{T}_\alpha$, sharing the selected vertex $\mathbf{v}_\alpha$. The inner sum runs over faces $f_\alpha \in \partial t_\alpha$ of each tetrahedron t_α. As already discussed in Section 6.1.1, in the latter sum the delta-function contributions vanish on the outer boundary of the set $\partial \mathcal{T}_\alpha$ and cancel pairwise for interior facets f_α, although not for the boundary facets ($f_\alpha \in \partial\Omega$). Therefore, Eq.(6.60) reduces to

$$\partial^i \phi_{\mathbf{v}_\alpha}(\mathbf{r}) = -\sum_{t_\alpha \in \mathcal{T}_\alpha} \frac{1}{h_{\mathbf{v}_\alpha, t_\alpha}} \hat{n}^i_{\mathbf{v}_\alpha, t_\alpha} \, \chi_{t_\alpha}(\mathbf{r}) - \sum_{f_\alpha \in \mathcal{F}_\alpha \cap \partial\Omega} \hat{n}^i_{f_\alpha, t_\alpha} \, \delta_{f_\alpha}(\mathbf{r}) \, \phi_{\mathbf{v}_\alpha, f_\alpha}(\mathbf{r}) , \tag{6.61}$$

where $\mathcal{F}_\alpha$ is the set of facets sharing the vertex $\mathbf{v}_\alpha$.

The term $A^{(c)}$ involves only the basis function $\boldsymbol{\psi}_{\mathbf{v}_\alpha,m}$, i.e., according to Eqs. (6.1) and (6.2), is given by

$$\phi_{\mathbf{v}_\alpha}(\mathbf{r}) = \sum_{t_\alpha \in \mathcal{T}_\alpha} \left[1 - \frac{1}{h_{\mathbf{v}_\alpha, t_\alpha}} \hat{\mathbf{n}}_{\mathbf{v}_\alpha, t_\alpha} \cdot (\mathbf{r} - \mathbf{v}_\alpha) \right] \chi_{t_\alpha}(\mathbf{r}) , \tag{6.62}$$

where $\chi_{t_\alpha}(\mathbf{r})$ is the characteristic function of the tetrahedron t_α. This basis function is multiplied by the gradient of the inverse density, which is proportional to a surface delta function on each facet on which the density is discontinuous. In the matrix element $A^{(c)}$

such delta-function contributions arise on facets shared by the tetrahedra t_α and t_β (the tetrahedra may be identical).

In both of the terms $A^{(b)}$ and $A^{(c)}$ the basis function $\phi_{\mathbf{v}_\beta}$ appears only through the expression

$$\begin{aligned}\Xi_{im}(\boldsymbol{\psi}_{\mathbf{v}_\beta,n}(\mathbf{r})) &:= \big(1-\xi_\lambda(\mathbf{r})\big)\,\delta_{im}\,\partial^l\,\boldsymbol{\psi}^l_{\mathbf{v}_\beta,n}(\mathbf{r}) - \xi_\mu(\mathbf{r})\,\big(\partial^i\,\boldsymbol{\psi}^m_{\mathbf{v}_\beta,n}(\mathbf{r}) + \partial^m\,\boldsymbol{\psi}^i_{\mathbf{v}_\beta,n}(\mathbf{r})\big)\\ &\equiv \big[\big(1-\xi_\lambda(\mathbf{r})\big)\,\delta_{nl}\,\delta_{im} - \xi_\mu(\mathbf{r})\,\big(\delta_{ni}\,\delta_{lm} + \delta_{nm}\,\delta_{li}\big)\big]\,\big(\partial^l\,\phi_{\mathbf{v}_\beta}(\mathbf{r})\big)\end{aligned} \tag{6.63}$$

(see Eq.(6.10)), which is related to the stress tensor σ_{im} associated with the basis function $\boldsymbol{\psi}_{\mathbf{v}_\beta,n}(\mathbf{r})$.

Eq.(6.63) has to be represented, by using Eqs. (6.1), (6.2), and (6.3), in terms of the basis functions $\phi_{\mathbf{v},\,t}$ supported on the individual tetrahedra. The result is

$$\begin{aligned}\Xi_{im}(\boldsymbol{\psi}_{\mathbf{v}_\beta,n}(\mathbf{r})) &= \sum_{t_\beta\in\mathcal{T}_\beta} X_{imnl}(t_\beta)\,\partial^l\,\phi_{\mathbf{v}_\beta,\,t_\beta}(\mathbf{r})\\ &\equiv -\sum_{t_\beta\in\mathcal{T}_\beta} X_{imnl}(t_\beta)\left[\frac{1}{h_{\mathbf{v}_\beta,\,t_\beta}}\,\hat{n}^l_{\mathbf{v}_\beta,\,t_\beta}\,\chi_{t_\beta}(\mathbf{r}) + \sum_{f_\beta\in\partial t_\beta}\phi_{\mathbf{v}_\beta,\,f_\beta}(\mathbf{r})\,\hat{n}^l_{f_\beta,\,t_\beta}\,\delta_{f_\beta}(\mathbf{r})\right],\end{aligned} \tag{6.64}$$

where

$$X_{imnl}(t_\beta) := \big(1-\xi_\lambda(t_\beta)\big)\,\delta_{im}\,\delta_{nl} + \xi_\mu(t_\beta)\,\big(\delta_{in}\,\delta_{ml} + \delta_{il}\,\delta_{mn}\big)\,, \tag{6.65}$$

and $\xi_\lambda(t_\beta)$ and $\xi_\mu(t_\beta)$ are the values of the coefficients ξ_λ and ξ_μ on the tetrahedron t_β. It is worth noting here that, by construction, the coefficients X_{imnl} have the same symmetry properties (Eq.(3.12)) as the general elasticity tensor for an anisotropic medium

$$X_{imnl} = X_{minl}\ ,\quad X_{imnl} = X_{imln}\ ,\quad X_{imnl} = X_{nlim}\ . \tag{6.66}$$

We will use this property in the following. A related remark is that the manipulation we are carrying out now could be probably generalized to anisotropic media, and the resulting stiffness matrix would have a similar structure to that in the present case.

By changing the order of summation, Eq.(6.64) can be recast in the form

$$\begin{aligned}&\Xi_{im}(\boldsymbol{\psi}_{\mathbf{v}_\beta,n}(\mathbf{r}))\\ &\quad= -\sum_{t_\beta\in\mathcal{T}_\beta} X_{imnl}(t_\beta)\,\frac{1}{h_{\mathbf{v}_\beta,\,t_\beta}}\,\hat{n}^l_{\mathbf{v}_\beta,\,t_\beta}\,\chi_{t_\beta}(\mathbf{r})\\ &\qquad-\sum_{f_\beta\in\mathcal{F}_\beta}\phi_{\mathbf{v}_\beta,\,f_\beta}(\mathbf{r})\,\delta_{f_\beta}(\mathbf{r})\sum_{t_\beta\in\mathcal{T}_{f_\beta}} X_{imnl}(t_\beta)\,\hat{n}^l_{f_\beta,\,t_\beta}\ ,\end{aligned} \tag{6.67}$$

where $\mathcal{T}_{f_\beta}$ is the set of (up to two) tetrahedra sharing the facet f_β. The last sum in Eq.(6.67) is thus, in general, a difference of two terms associated with the tetrahedra adjacent to the given face f_β. Therefore, we can write Eq.(6.67) as

$$\begin{aligned}&\Xi_{im}(\boldsymbol{\psi}_{\mathbf{v}_\beta,n}(\mathbf{r}))\\ &\quad= -\sum_{t_\beta\in\mathcal{T}_\beta} X_{imnl}(t_\beta)\,\frac{1}{h_{\mathbf{v}_\beta,\,t_\beta}}\,\hat{n}^l_{\mathbf{v}_\beta,\,t_\beta}\,\chi_{t_\beta}(\mathbf{r})\\ &\qquad-\sum_{f_\beta\in\mathcal{F}_\beta\cap\partial\Omega}\big[X_{imnl}(t_\beta+) - X_{imnl}(t_\beta-)\big]\,\hat{n}^l_{f_\beta}\,\delta_{f_\beta}(\mathbf{r})\,\phi_{\mathbf{v}_\beta,\,f_\beta}(\mathbf{r})\ ,\end{aligned} \tag{6.68}$$

where $t_\beta+$ and $t_\beta-$ are tetrahedra on the positive and negative sides of the facet f_β (relative to the direction of the normal $\hat{\mathbf{n}}_{f_\beta}$ to the face). We also used here the fact (discussed in connection with Eq.(6.61)) that the delta-function contributions cancel pairwise on all facets f_β except those located on the exterior object boundary $\partial\Omega$.

Finally, we note that we can drop the delta-function contributions (i.e., the second sum in Eq.(6.69)), altogether: the reason is that we can think of the object boundary $\partial\Omega$ as an interface between the object and the external region discretized with "fictitious" tetrahedra having properties of the background medium ($\xi_\lambda = 1$ and $\xi_\mu = 0$, hence $X = 0$). With this interpretation, the surface $\partial\Omega$ is no longer a boundary (we have used a similar argument in acoustics). Hence, we have, eventually,

$$\Xi_{im}(\boldsymbol{\psi}_{\mathbf{v}_\beta,n}(\mathbf{r})) = -\sum_{t_\beta \in \mathcal{T}_\beta} X_{imnl}(t_\beta)\, \frac{1}{h_{\mathbf{v}_\beta,\,t_\beta}}\, \hat{n}^l_{\mathbf{v}_\beta,\,t_\beta}\, \chi_{t_\beta}(\mathbf{r})\ . \tag{6.69}$$

It will be also useful to introduce a quantity related directly to the stress tensor,

$$\Sigma_{im}(\boldsymbol{\psi}_{\mathbf{v}_\beta,n}(\mathbf{r})) := \frac{1}{\lambda_0}\, \sigma_{im}(\boldsymbol{\psi}_{\mathbf{v}_\beta,n}(\mathbf{r}))\ , \tag{6.70}$$

which can be represented, in analogy to Eq.(6.69), as

$$\begin{aligned} &\Sigma_{im}(\boldsymbol{\psi}_{\mathbf{v}_\beta,n}(\mathbf{r})) \\ &\quad= -\sum_{t_\beta \in \mathcal{T}_\beta} E_{imnl}(t_\beta)\, \frac{1}{h_{\mathbf{v}_\beta,\,t_\beta}}\, \hat{n}^l_{\mathbf{v}_\beta,\,t_\beta}\, \chi_{t_\beta}(\mathbf{r}) \\ &\qquad - \sum_{f_\beta \in \mathcal{F}_\beta \cap \partial\Omega} \big[E_{imnl}(t_\beta+) - E_{imnl}(t_\beta-)\big]\, \hat{n}^l_{f_\beta}\, \delta_{f_\beta}(\mathbf{r})\, \phi_{\mathbf{v}_\beta,\,f_\beta}(\mathbf{r})\ , \end{aligned} \tag{6.71}$$

where

$$E_{imnl}(t_\beta) := \eta_\lambda(t_\beta)\, \delta_{im}\, \delta_{nl} + \eta_\mu(t_\beta)\, \big(\delta_{in}\, \delta_{ml} + \delta_{il}\, \delta_{mn}\big)\ , \tag{6.72}$$

and

$$\eta_\lambda(t_\beta) := \frac{\rho(t_\beta)}{\rho_0}\, \xi_\lambda(t_\beta) = \frac{\lambda(t_\beta)}{\lambda_0}\ , \qquad \eta_\mu(t_\beta) := \frac{\rho(t_\beta)}{\rho_0}\, \xi_\mu(t_\beta) = \frac{\mu(t_\beta)}{\lambda_0} \tag{6.73}$$

(cf. Eqs. (3.10) and (3.11)). The expression $\Sigma_{im}(\boldsymbol{\psi}_{\mathbf{v}_\beta,n}(\mathbf{r}))$ appears in the matrix element $A^{(c)}$.

In terms of the tensors (6.63) and (6.70), the contributions to the matrix elements are then given simply by

$$A^{(b)}_{\mathbf{v}_\alpha,m;\mathbf{v}_\beta,n} = -\,k^{-2} \int \mathrm{d}^3r\, \big(\partial^i \phi_{\mathbf{v}_\alpha}(\mathbf{r})\big)\, \Xi_{im}(\boldsymbol{\psi}_{\mathbf{v}_\beta,n}(\mathbf{r})) \tag{6.74}$$

and

$$A^{(c)}_{\mathbf{v}_\alpha,m;\mathbf{v}_\beta,n} = -\,k^2 \int \mathrm{d}^3r\, \phi_{\mathbf{v}_\alpha}(\mathbf{r}) \left(\partial^i \frac{\rho_0}{\rho(\mathbf{r})}\right) \Sigma_{im}(\boldsymbol{\psi}_{\mathbf{v}_\beta,n}(\mathbf{r}))\ . \tag{6.75}$$

The terms $A^{(d)}$ and $A^{(e)}$: The remaining terms in the matrix elements involve several common expressions:

Second derivatives of the basis function ϕ_α. These expressions (Eq.(6.8)) were given in Section 6.1.1. Clearly, they cannot be used directly in evaluating the matrix elements: derivatives of the delta function have to be eliminated in favor of derivatives of the Green function. We will carry out this rearrangement in the following.

The stress tensor associated with the basis function $\phi_{\mathbf{v}_\beta}$. In Eqs. (6.59d) and (6.59e) the basis function $\phi_{\mathbf{v}_\beta}$ appears only through the quantity

$$\begin{aligned}\Xi_{ij}(\boldsymbol{\psi}_{\mathbf{v}_\beta,n}(\mathbf{r})) &:= \xi_\lambda(\mathbf{r})\,\delta_{ij}\,\partial^l\,\boldsymbol{\psi}^l_{\mathbf{v}_\beta,n}(\mathbf{r}) + \xi_\mu(\mathbf{r})\left(\partial^i\,\boldsymbol{\psi}^j_{\mathbf{v}_\beta,n}(\mathbf{r}) + \partial^j\,\boldsymbol{\psi}^i_{\mathbf{v}_\beta,n}(\mathbf{r})\right)\\ &\equiv \left[\left(1-\xi_\lambda(\mathbf{r})\right)\delta_{nl}\,\delta_{ij} - \xi_\mu(\mathbf{r})\left(\delta_{ni}\,\delta_{lj} + \delta_{nj}\,\delta_{li}\right)\right]\left(\partial^l\,\phi_{\mathbf{v}_\beta}(\mathbf{r})\right)\end{aligned} \tag{6.76}$$

(cf. Eq.(6.63)), related to the stress tensor σ_{ij} associated with the basis function $\boldsymbol{\psi}_{\mathbf{v}_\beta,n}(\mathbf{r})$. It can be expressed, as in Eq.(6.69), in terms of constant basis functions supported on the tetrahedra.

Similarly to Eqs. (6.74) and (6.75), Eqs. (6.59d) and (6.59e) take the form

$$\begin{aligned}A^{(d)}_{\mathbf{v}_\alpha,m;\mathbf{v}_\beta,n} = k^{-2}\int \mathrm{d}^3r_1 \int \mathrm{d}^3r_2\,&\left(\partial_1^m\,\partial_1^i\,\phi_{\mathbf{v}_\alpha}(\mathbf{r}_1)\right)\left(\partial_1^j\,g(\mathbf{r}_1-\mathbf{r}_2)\right)\\ &\Xi_{ij}(\boldsymbol{\psi}_{\mathbf{v}_\beta,n}(\mathbf{r}_2))\end{aligned} \tag{6.77}$$

and

$$\begin{aligned}A^{(e)}_{\mathbf{v}_\alpha,m;\mathbf{v}_\beta,n} = k^{-2}\int \mathrm{d}^3r_1 \int \mathrm{d}^3r_2\,&\left(\partial_1^m\,\partial_1^i\,\phi_{\mathbf{v}_\alpha}(\mathbf{r}_1)\right) g(\mathbf{r}_1-\mathbf{r}_2)\\ &\left(\partial_2^j\frac{\rho_0}{\rho(\mathbf{r}_2)}\right)\Sigma_{ij}(\boldsymbol{\psi}_{\mathbf{v}_\beta,n}(\mathbf{r}_2))\ .\end{aligned} \tag{6.78}$$

Full expressions for $A^{(d)}$ and $A^{(e)}$. After substituting Eq.(6.8) in Eq.(6.77) we integrate one of the terms by parts in order to eliminate the derivatives of the delta function in the expression for the derivatives of the basis function $\phi_{\mathbf{v}_\alpha}$. We obtain, instead, an additional derivative of the Green function contracted with the normals to the facets on which the derivative of $\phi_{\mathbf{v}_\alpha}$ is supported ($\hat{n}^p_{f_\alpha}\,\partial_1^p\,g(\mathbf{r}_1-\mathbf{r}_2)$ in the third term of Eq.(6.79)

below). The result is

$$
\begin{aligned}
&A^{(d)}_{\mathbf{v}_\alpha,m;\mathbf{v}_\beta,n} \\
&= -\,2\,k^{-2} \sum_{f_\alpha\in\mathcal{F}_\alpha} \left(\frac{\hat{\mathbf{n}}_{\mathbf{v}_\alpha,\,t_\alpha+}\cdot\hat{\mathbf{n}}_{f_\alpha}}{h_{\mathbf{v}_\alpha,\,t_\alpha+}} - \frac{\hat{\mathbf{n}}_{\mathbf{v}_\alpha,\,t_\alpha-}\cdot\hat{\mathbf{n}}_{f_\alpha}}{h_{\mathbf{v}_\alpha,\,t_\alpha-}} \right) \hat{n}^m_{f_\alpha}\,\hat{n}^i_{f_\alpha} \\
&\qquad\qquad \int_{f_\alpha} \mathrm{d}^2r_1 \int \mathrm{d}^3r_2 \left(\partial^j_1\, g(\mathbf{r}_1-\mathbf{r}_2)\right) \Xi_{ij}(\boldsymbol{\psi}_{\mathbf{v}_\beta,n}(\mathbf{r}_2)) \\
&\quad +\,2\,k^{-2} \sum_{f_\alpha\in\partial\mathcal{T}_\alpha} \frac{1}{h_{\mathbf{v}_\alpha,\,t_\alpha}}\,\hat{n}^m_{f_\alpha}\,\hat{n}^i_{f_\alpha} \\
&\qquad\qquad \int_{f_\alpha} \mathrm{d}^2r_1 \int \mathrm{d}^3r_2 \left(\partial^j_1\, g(\mathbf{r}_1-\mathbf{r}_2)\right) \Xi_{ij}(\boldsymbol{\psi}_{\mathbf{v}_\beta,n}(\mathbf{r}_2)) \\
&\quad +\,k^{-2} \sum_{f_\alpha\in\mathcal{F}_\alpha\cap\,\partial\Omega} \hat{n}^m_{f_\alpha}\,\hat{n}^i_{f_\alpha}\,\hat{n}^p_{f_\alpha} \\
&\qquad\qquad \int_{f_\alpha} \mathrm{d}^2r_1 \int \mathrm{d}^3r_2 \left(\partial^j_1\,\partial^p_1\, g(\mathbf{r}_1-\mathbf{r}_2)\right) \Xi_{ij}(\boldsymbol{\psi}_{\mathbf{v}_\beta,n}(\mathbf{r}_2))\ .
\end{aligned}
\tag{6.79}
$$

Similarly, we obtain

$$
\begin{aligned}
&A^{(e)}_{\mathbf{v}_\alpha,m;\mathbf{v}_\beta,n} \\
&= 2\,k^{-2} \sum_{f_\alpha\in\mathcal{F}_\alpha} \left(\frac{\hat{\mathbf{n}}_{\mathbf{v}_\alpha,\,t_\alpha+}\cdot\hat{\mathbf{n}}_{f_\alpha}}{h_{\mathbf{v}_\alpha,\,t_\alpha+}} - \frac{\hat{\mathbf{n}}_{\mathbf{v}_\alpha,\,t_\alpha-}\cdot\hat{\mathbf{n}}_{f_\alpha}}{h_{\mathbf{v}_\alpha,\,t_\alpha-}} \right) \hat{n}^m_{f_\alpha}\,\hat{n}^i_{f_\alpha} \\
&\qquad\qquad \int_{f_\alpha} \mathrm{d}^2r_1 \int \mathrm{d}^3r_2\, g(\mathbf{r}_1-\mathbf{r}_2) \left(\partial^j_2 \frac{\rho_0}{\rho(\mathbf{r}_2)}\right) \Sigma_{ij}(\boldsymbol{\psi}_{\mathbf{v}_\beta,n}(\mathbf{r}_2)) \\
&\quad -\,2\,k^{-2} \sum_{f_\alpha\in\partial\mathcal{T}_\alpha} \frac{1}{h_{\mathbf{v}_\alpha,\,t_\alpha}}\,\hat{n}^m_{f_\alpha}\,\hat{n}^i_{f_\alpha} \\
&\qquad\qquad \int_{f_\alpha} \mathrm{d}^2r_1 \int \mathrm{d}^3r_2\, g(\mathbf{r}_1-\mathbf{r}_2) \left(\partial^j_2 \frac{\rho_0}{\rho(\mathbf{r}_2)}\right) \Sigma_{ij}(\boldsymbol{\psi}_{\mathbf{v}_\beta,n}(\mathbf{r}_2)) \\
&\quad -\,k^{-2} \sum_{f_\alpha\in\mathcal{F}_\alpha\cap\,\partial\Omega} \hat{n}^m_{f_\alpha}\,\hat{n}^i_{f_\alpha}\,\hat{n}^p_{f_\alpha} \\
&\qquad\qquad \int_{f_\alpha} \mathrm{d}^2r_1 \int \mathrm{d}^3r_2 \left(\partial^p_1\, g(\mathbf{r}_1-\mathbf{r}_2)\right) \left(\partial^j_2 \frac{\rho_0}{\rho(\mathbf{r}_2)}\right) \Sigma_{ij}(\boldsymbol{\psi}_{\mathbf{v}_\beta,n}(\mathbf{r}_2))\ .
\end{aligned}
\tag{6.80}
$$

Finally, by substituting Eq.(6.69) in Eq.(6.79), we obtain a sum of several terms, involv-

ing integrals over tetrahedra and facets,

$$
\begin{aligned}
&A^{(d)}_{\mathbf{v}_\alpha,m;\mathbf{v}_\beta,n} \\
&= 2\,k^{-2} \sum_{f_\alpha\in\mathcal{F}_\alpha} \sum_{t_\beta\in\mathcal{T}_\beta} \left(\frac{\hat{\mathbf{n}}_{\mathbf{v}_\alpha,\,t_\alpha+}\cdot\hat{\mathbf{n}}_{f_\alpha}}{h_{\mathbf{v}_\alpha,\,t_\alpha+}} - \frac{\hat{\mathbf{n}}_{\mathbf{v}_\alpha,\,t_\alpha-}\cdot\hat{\mathbf{n}}_{f_\alpha}}{h_{\mathbf{v}_\alpha,\,t_\alpha-}} \right) \hat{n}^m_{f_\alpha}\,\hat{n}^i_{f_\alpha} \\
&\qquad X_{ijnl}(t_\beta)\,\frac{1}{h_{\mathbf{v}_\beta,\,t_\beta}}\,\hat{n}^l_{\mathbf{v}_\beta,\,t_\beta} \\
&\qquad \int_{f_\alpha} \mathrm{d}^2 r_1 \int_{t_\beta} \mathrm{d}^3 r_2\,\partial^j_1\,g(\mathbf{r}_1-\mathbf{r}_2) \\
&- 2\,k^{-2} \sum_{f_\alpha\in\partial\mathcal{T}_\alpha} \sum_{t_\beta\in\mathcal{T}_\beta} \frac{1}{h_{\mathbf{v}_\alpha,\,t_\alpha}}\,\hat{n}^m_{f_\alpha}\,\hat{n}^i_{f_\alpha}\,X_{ijnl}(t_\beta)\,\frac{1}{h_{\mathbf{v}_\beta,\,t_\beta}}\,\hat{n}^l_{\mathbf{v}_\beta,\,t_\beta} \\
&\qquad \int_{f_\alpha} \mathrm{d}^2 r_1 \int_{t_\beta} \mathrm{d}^3 r_2\,\partial^j_1\,g(\mathbf{r}_1-\mathbf{r}_2) \\
&- k^{-2} \sum_{f_\alpha\in\mathcal{F}_\alpha\cap\,\partial\Omega} \sum_{t_\beta\in\mathcal{T}_\beta} \hat{n}^m_{f_\alpha}\,\hat{n}^i_{f_\alpha}\,\hat{n}^k_{f_\alpha}\,X_{ijnl}(t_\beta)\,\frac{1}{h_{\mathbf{v}_\beta,\,t_\beta}}\,\hat{n}^l_{\mathbf{v}_\beta,\,t_\beta} \\
&\qquad \int_{f_\alpha} \mathrm{d}^2 r_1 \int_{t_\beta} \mathrm{d}^3 r_2\,\partial^j_1\,\partial^k_1\,g(\mathbf{r}_1-\mathbf{r}_2)\ .
\end{aligned}
\tag{6.81}
$$

Similarly, Eq.(6.71) substituted in Eq.(6.80) yields

$$
\begin{aligned}
&A^{(e)}_{\mathbf{v}_\alpha,m;\mathbf{v}_\beta,n} \\
&= 2\,k^{-2} \sum_{f_\alpha\in\mathcal{F}_\alpha} \sum_{t_\beta\in\mathcal{T}_\beta} \sum_{f_\beta\in\partial t_\beta} \left(\frac{\hat{\mathbf{n}}_{\mathbf{v}_\alpha,\,t_\alpha+}\cdot\hat{\mathbf{n}}_{f_\alpha}}{h_{\mathbf{v}_\alpha,\,t_\alpha+}} - \frac{\hat{\mathbf{n}}_{\mathbf{v}_\alpha,\,t_\alpha-}\cdot\hat{\mathbf{n}}_{f_\alpha}}{h_{\mathbf{v}_\alpha,\,t_\alpha-}} \right) \hat{n}^m_{f_\alpha}\,\hat{n}^i_{f_\alpha} \\
&\qquad \left(\frac{\rho_0}{\rho(f_\beta+)} - \frac{\rho_0}{\rho(f_\beta-)} \right) E_{ijnl}(t_\beta)\,\frac{1}{h_{\mathbf{v}_\beta,\,t_\beta}}\,\hat{n}^j_{f_\beta,\,t_\beta}\,\hat{n}^l_{\mathbf{v}_\beta,\,t_\beta} \\
&\qquad \int_{f_\alpha} \mathrm{d}^2 r_1 \int_{f_\beta} \mathrm{d}^2 r_2\,g(\mathbf{r}_1-\mathbf{r}_2) \\
&- 2\,k^{-2} \sum_{f_\alpha\in\partial\mathcal{T}_\alpha} \sum_{t_\beta\in\mathcal{T}_\beta} \sum_{f_\beta\in\partial t_\beta} \frac{1}{h_{\mathbf{v}_\alpha,\,t_\alpha}}\,\hat{n}^m_{f_\alpha}\,\hat{n}^i_{f_\alpha} \\
&\qquad \left(\frac{\rho_0}{\rho(f_\beta+)} - \frac{\rho_0}{\rho(f_\beta-)} \right) E_{ijnl}(t_\beta)\,\frac{1}{h_{\mathbf{v}_\beta,\,t_\beta}}\,\hat{n}^j_{f_\beta,\,t_\beta}\,\hat{n}^l_{\mathbf{v}_\beta,\,t_\beta} \\
&\qquad \int_{f_\alpha} \mathrm{d}^2 r_1 \int_{f_\beta} \mathrm{d}^2 r_2\,g(\mathbf{r}_1-\mathbf{r}_2) \\
&- k^{-2} \sum_{f_\alpha\in\mathcal{F}_\alpha\cap\,\partial\Omega} \sum_{t_\beta\in\mathcal{T}_\beta} \sum_{f_\beta\in\partial t_\beta} \hat{n}^m_{f_\alpha}\,\hat{n}^i_{f_\alpha}\,\hat{n}^k_{f_\alpha} \\
&\qquad \left(\frac{\rho_0}{\rho(f_\beta+)} - \frac{\rho_0}{\rho(f_\beta-)} \right) E_{ijnl}(t_\beta)\,\frac{1}{h_{\mathbf{v}_\beta,\,t_\beta}}\,\hat{n}^j_{f_\beta,\,t_\beta}\,\hat{n}^l_{\mathbf{v}_\beta,\,t_\beta} \\
&\qquad \int_{f_\alpha} \mathrm{d}^2 r_1 \int_{f_\beta} \mathrm{d}^2 r_2\,\partial^k_1\,g(\mathbf{r}_1-\mathbf{r}_2)\ .
\end{aligned}
\tag{6.82}
$$

By reversing the order of summation, the above expression can be written as

$$
\begin{aligned}
& A^{(e)}_{\mathbf{v}_\alpha,m;\mathbf{v}_\beta,n} \\
& = \; 2\,k^{-2} \sum_{f_\alpha \in \mathcal{F}_\alpha} \sum_{f_\beta \in \partial \mathcal{T}_\beta} \left(\frac{\hat{\mathbf{n}}_{\mathbf{v}_\alpha,\,t_\alpha +} \cdot \hat{\mathbf{n}}_{f_\alpha}}{h_{\mathbf{v}_\alpha,\,t_\alpha +}} - \frac{\hat{\mathbf{n}}_{\mathbf{v}_\alpha,\,t_\alpha -} \cdot \hat{\mathbf{n}}_{f_\alpha}}{h_{\mathbf{v}_\alpha,\,t_\alpha -}} \right) \hat{n}^m_{f_\alpha}\,\hat{n}^i_{f_\alpha} \\
& \qquad\qquad\qquad \left(\frac{\rho_0}{\rho(t_\beta +)} - \frac{\rho_0}{\rho(t_\beta -)} \right) E_{ijnl}(t_\beta)\,\frac{1}{h_{\mathbf{v}_\beta,\,t_\beta}}\,\hat{n}^j_{f_\beta,\,t_\beta}\,\hat{n}^l_{\mathbf{v}_\beta,\,t_\beta} \\
& \qquad\qquad\qquad \int_{f_\alpha} \mathrm{d}^2 r_1 \int_{f_\beta} \mathrm{d}^2 r_2\, g(\mathbf{r}_1 - \mathbf{r}_2) \\
& - \; 2\,k^{-2} \sum_{f_\alpha \in \partial \mathcal{T}_\alpha} \sum_{f_\beta \in \partial \mathcal{T}_\beta} \frac{1}{h_{\mathbf{v}_\alpha,\,t_\alpha}}\,\hat{n}^m_{f_\alpha}\,\hat{n}^i_{f_\alpha} \\
& \qquad\qquad\qquad \left(\frac{\rho_0}{\rho(t_\beta +)} - \frac{\rho_0}{\rho(t_\beta -)} \right) E_{ijnl}(t_\beta)\,\frac{1}{h_{\mathbf{v}_\beta,\,t_\beta}}\,\hat{n}^j_{f_\beta,\,t_\beta}\,\hat{n}^l_{\mathbf{v}_\beta,\,t_\beta} \\
& \qquad\qquad\qquad \int_{f_\alpha} \mathrm{d}^2 r_1 \int_{f_\beta} \mathrm{d}^2 r_2\, g(\mathbf{r}_1 - \mathbf{r}_2) \\
& - \; k^{-2} \sum_{f_\alpha \in \mathcal{F}_\alpha \cap \partial\Omega} \sum_{f_\beta \in \partial \mathcal{T}_\beta} \hat{n}^m_{f_\alpha}\,\hat{n}^i_{f_\alpha}\,\hat{n}^k_{f_\alpha} \\
& \qquad\qquad\qquad \left(\frac{\rho_0}{\rho(t_\beta +)} - \frac{\rho_0}{\rho(t_\beta -)} \right) E_{ijnl}(t_\beta)\,\frac{1}{h_{\mathbf{v}_\beta,\,t_\beta}}\,\hat{n}^j_{f_\beta,\,t_\beta}\,\hat{n}^l_{\mathbf{v}_\beta,\,t_\beta} \\
& \qquad\qquad\qquad \int_{f_\alpha} \mathrm{d}^2 r_1 \int_{f_\beta} \mathrm{d}^2 r_2\, \partial^k_1\, g(\mathbf{r}_1 - \mathbf{r}_2) \; .
\end{aligned}
\tag{6.83}
$$

All the contributions to the $\mathbf{r}_2$-integrals in Eq.(6.82) come from discontinuities of the inverse density, $\rho_0/\rho(f_\beta+) - \rho_0/\rho(f_\beta-)$, where $\rho(f_\beta+)$ and $\rho(f_\beta-)$ are densities in tetrahedra on the positive and negative sides of the face f_β, as defined by the normal $\hat{\mathbf{n}}_{f_\beta,t_\beta}$ (which is, by definition, exterior to the tetrahedron t_β).

In the alternative expression Eq.(6.83) come from discontinuities of the inverse density,

6.3.5 Summary of the expressions for the "basic" matrix elements

The fundamental matrix elements, required in the computation of the matrix elements the second-order formulation are listed in the following. Symbols (d) and (e) indicate the contribution in which the given matrix element appears.

tetrahedron-facet matrix elements:

constant-constant:

TF2(d) $A^i(t_\alpha; f_\beta) = \int_{t_\alpha} \mathrm{d}^3 r_1 \int_{f_\beta} \mathrm{d}^2 r_2\, \partial^i\, g(\mathbf{r}_1 - \mathbf{r}_2)$

TF3(d) $A^i_{\mathrm{n}}(t_\alpha; f_\beta) = \hat{n}^j_{f_\beta} \int_{t_\alpha} \mathrm{d}^3 r_1 \int_{f_\beta} \mathrm{d}^2 r_2\, \partial^i\, \partial^j\, g(\mathbf{r}_1 - \mathbf{r}_2)$

facet-facet matrix elements:

constant-constant:

FF1(e) $A(f_\alpha; f_\beta) = \int_{f_\alpha} \mathrm{d}^2 r_1 \int_{f_\beta} \mathrm{d}^2 r_2\, g(\mathbf{r}_1 - \mathbf{r}_2)$

FF2(e) $A_\mathrm{n}(f_\alpha; f_\beta) = \hat{n}^i_{f_\alpha} \int_{f_\alpha} \mathrm{d}^2 r_1 \int_{f_\beta} \mathrm{d}^2 r_2\, \partial^i g(\mathbf{r}_1 - \mathbf{r}_2)$

The subscript "n" in $A_\mathrm{n}(\cdot)$ is used to indicate matrix elements involving the normal derivative of the Green function.

6.4 Representation of matrix elements

We recast here matrix elements evaluated in the previous Subsections in a general representation used in the following in computation of the compressed stiffness matrix. This purpose of using this representation is to facilitate programming and allow an efficient ordering of operations in the matrix construction stage (as described in Section 6.6).

We give here a somewhat schematic expression for the matrix – the details of its implementation will be given in Section 6.6.

The representation has an almost factorized form[2]

$$\begin{aligned} A^{(\nu)}_{\alpha\beta} &= \sum_{\nu_1\,\nu_2} B_{\nu\,\nu_1\,\nu_2} \\ &\int \mathrm{d}r_1 \int \mathrm{d}r_2\, C^{(1\,\nu_1)\,I_1}_{\alpha;\,M_1}\, \phi_{M_1}(\mathbf{r}_1) \left[\mathcal{D}^{I_1\,I_2}\, g(\mathbf{r}_1 - \mathbf{r}_2)\right] \phi_{M_2}(\mathbf{r}_2)\, C^{(2\,\nu_2)\,I_2}_{\beta;\,M_2}\ . \end{aligned} \tag{6.84}$$

In this expression:

1. The indices α and β are unknown numbers.

2. The indices ν_j, $j = 1, 2$, label specific contributions to the matrix. In the practical implementation they are simply integers uniquely identifying the given contribution to the matrix and the given coefficient C.

3. The matrix B is a set of coefficients 0 or 1 indicating which contributions are included in the sum.

4. The multi-indices M_j, $j = 1, 2$ (generally, M) label the "fundamental" basis functions ϕ_M. In the present case, they are constant or linear basis functions supported on tetrahedra or facets.

5. The operators $\mathcal{D}^{I_1\,I_2}$ are differential operators representing partial derivatives specified by the (multi-)indices I, acting on the scalar Green function g. In practice, derivatives only up to the second order will appear.

[2]Full factorization does not seem possible, because some matrix elements are modified by hand through integration by parts and similar manipulations.

6. The coefficients $C^{(j\,\nu_j)\,I_j}_{\alpha;\,M_j}$ provide a link between the unknowns and the basis functions. The indices ν_j are additional labels indexing possible types of unknowns. In general, the coefficients C (especially $C^{(2)}$) will depend on the material parameters. In the following we consider a given set $C^{(j\,\nu_j)\,\cdot}_{\dots;\,\dots}$ of coefficients as a sparse matrix whose rows are labeled by the unknowns α.

In addition to the coefficients C (which provide a mapping from the unknowns to the fundamental basis functions), we also need an "inverse" mapping D from the fundamental basis functions to the unknowns. As we discuss later, these mapping are used in the matrix assembly.

The idea of the representation (6.84) is to provide a universal scheme for matrix element computation, and allow full flexibility in defining and modifying the form of the integral equations.

Sets of the coefficients C are precomputed and then supplied as arguments to an "assembly" routine, which constructs contributions to the output matrix elements from the "basic" matrix elements defined in terms of the "fundamental" basis functions and the Green function or its derivatives. The same coefficients are used in evaluation of the MoM-Cartesian mapping coefficients V, as the mapping of unknowns will be expressed in terms of mappings of the fundamental basis functions.

The coefficients C are also incorporates as a component in the compressed stiffness matrix. The reason is that elements of the map V_α for the unknowns may be linear combinations of many map elements for the fundamental basis functions; therefore, it is more economical to store those basic mappings and convert the MoM variables into equivalent sources (and vice versa) in two stages.

In the above description we assumed that the far-field part of the matrix is represented not only in terms of the Green function, but also of its derivatives. However, this type of representation has to be carefully examined on the case-by-case basis, particularly from the point of view of storage. If we decide to use the Green function only, the far-field coefficients will be different than the coefficients C above; nevertheless, storage of the expansion of the mappings for the fundamental basis functions may be still more economical than for the unknowns.

In the expressions below the symbols $\mathrm{C}(t)$ and $\mathrm{C}(f)$ refer to functions constant on tetrahedra and facets, and $\mathrm{L}(\mathbf{v}, t)$ and $\mathrm{L}(\mathbf{v}, f)$ to functions linear on tetrahedra and facets; in the latter case, $\mathbf{v}$ is the selected vertex (at which the basis function has value 1). Extra overall coefficients are included in the B.

6.4.1 Matrix elements for second-order equations

We give here examples of expressions for the matrix elements in the second-order formulation of Eqs. (6.74), (6.75), (6.81), (6.82) (these are the most complicated ones).

We give alternative expressions for some coefficients C, differing by the presence of absence of one factor $\hat{n}\cdot$; those with the missing factor are used with basic matrix elements involving the normal derivative of the Green function. For notational simplicity, some of the constant coefficients are not displayed in these formulae, and are absorbed in the factors B appearing in Eq.(6.84).

The contribution $A^{(d)}$:

$$C^{(1\,e\,\mathrm{C})\,i}_{\mathbf{v}_\alpha,m;\,f_\alpha} = \left(\frac{\hat{\mathbf{n}}_{\mathbf{v}_\alpha,\,t_\alpha+}\cdot\hat{\mathbf{n}}_{f_\alpha}}{h_{\mathbf{v}_\alpha,\,t_\alpha+}} - \frac{\hat{\mathbf{n}}_{\mathbf{v}_\alpha,\,t_\alpha-}\cdot\hat{\mathbf{n}}_{f_\alpha}}{h_{\mathbf{v}_\alpha,\,t_\alpha-}}\right)\hat{n}^m_{f_\alpha}\,\hat{n}^i_{f_\alpha}\ , \qquad f_\alpha\in\mathcal{F}_\alpha\ , \tag{6.85a}$$

$$C^{(1\,e\,\mathrm{C})\,i}_{\mathbf{v}_\alpha,m;\,f_\alpha} = \frac{1}{h_{\mathbf{v}_\alpha,\,t_\alpha}}\,\hat{n}^m_{f_\alpha}\,\hat{n}^i_{f_\alpha}\ , \qquad f_\alpha\in\partial\mathcal{T}_\alpha\ , \tag{6.85b}$$

$$C^{(1\,e\,\mathrm{C})\,ik}_{\mathbf{v}_\alpha,m;\,f_\alpha} = \frac{1}{h_{\mathbf{v}_\alpha,\,t_\alpha}}\,\hat{n}^m_{f_\alpha}\,\hat{n}^i_{f_\alpha}\,\hat{n}^k_{f_\alpha}\ , \qquad f_\alpha\in\partial\mathcal{T}_\alpha\cap\partial\Omega\ , \tag{6.85c}$$

$$C^{(1\,e\,\mathrm{Cn})\,i}_{\mathbf{v}_\alpha,m;\,f_\alpha} = \frac{1}{h_{\mathbf{v}_\alpha,\,t_\alpha}}\,\hat{n}^m_{f_\alpha}\,\hat{n}^i_{f_\alpha}\ , \qquad f_\alpha\in\partial\mathcal{T}_\alpha\cap\partial\Omega\ , \tag{6.85d}$$

$$C^{(2\,e\,\mathrm{C})\,ij}_{\mathbf{v}_\beta,n;\,t_\beta} = X_{ijnl}(t_\beta)\,\frac{1}{h_{\mathbf{v}_\beta,\,t_\beta}}\,\hat{n}^l_{\mathbf{v}_\beta,\,t_\beta}\ , \qquad t_\beta\in\mathcal{T}_\beta\ , \tag{6.85e}$$

$$C^{(2\,e\,\mathrm{L})\,ij}_{\mathbf{v}_\beta,n;\,\mathbf{v}_\beta,\,f_\beta} = \left[X_{ijnl}(t_\beta+) - X_{ijnl}(t_\beta-)\right]\hat{n}^l_{f_\beta}\ , \qquad f_\beta\in\mathcal{F}_\beta\ . \tag{6.85f}$$

In terms of these coefficients, the matrix element (6.81), written in the form of Eq.(6.84),

is

$$
\begin{aligned}
A^{(d)}_{\mathbf{v}_\alpha,m;\mathbf{v}_\beta,n} &= \sum_{\nu_1\,\nu_2} B^{(dXX)}(\nu_1,\nu_2) \int \mathrm{d}r_1 \int \mathrm{d}r_2 \\
&\quad C^{(1\,e\,\nu_1)\,I_1}_{\mathbf{v}_\alpha,m;\,M_1}\,\phi_{M_1}(\mathbf{r}_1)\left[\mathcal{D}^{I_1\,I_2}\,g(\mathbf{r}_1-\mathbf{r}_2)\right]\phi_{M_2}(\mathbf{r}_2)\,C^{(2\,e\,\nu_2)\,I_2}_{\mathbf{v}_\beta,n;\,M_2} \\
&\quad = \int \mathrm{d}r_1 \int \mathrm{d}r_2 \\
&\quad \Big\{ C^{(1\,e\,\mathrm{C})\,i}_{\mathbf{v}_\alpha,m;\,f_\alpha}\,\chi_{f_\alpha}(\mathbf{r}_1)\left[\partial^j\,g(\mathbf{r}_1-\mathbf{r}_2)\right]\chi_{t_\beta}(\mathbf{r}_2)\,C^{(2\,e\,\mathrm{C})\,ij}_{\mathbf{v}_\beta,n;\,t_\beta} \\
&\quad + C^{(1\,e\,\mathrm{C})\,i}_{\mathbf{v}_\alpha,m;\,f_\alpha}\,\chi_{f_\alpha}(\mathbf{r}_1)\left[\partial^j\,g(\mathbf{r}_1-\mathbf{r}_2)\right]\phi_{\mathbf{v}_\beta,\,f_\beta}(\mathbf{r}_2)\,C^{(2\,e\,\mathrm{L})\,ij}_{\mathbf{v}_\beta,n;\,\mathbf{v}_\beta,\,f_\beta} \\
&\quad + C^{(1\,e\,\mathrm{C})\,i}_{\mathbf{v}_\alpha,m;\,f_\alpha}\,\chi_{f_\alpha}(\mathbf{r}_1)\left[\partial^j\,g(\mathbf{r}_1-\mathbf{r}_2)\right]\chi_{t_\beta}(\mathbf{r}_2)\,C^{(2\,e\,\mathrm{C})\,ij}_{\mathbf{v}_\beta,n;\,t_\beta} \\
&\quad + C^{(1\,e\,\mathrm{C})\,i}_{\mathbf{v}_\alpha,m;\,f_\alpha}\,\chi_{f_\alpha}(\mathbf{r}_1)\left[\partial^j\,g(\mathbf{r}_1-\mathbf{r}_2)\right]\phi_{\mathbf{v}_\beta,\,f_\beta}(\mathbf{r}_2)\,C^{(2\,e\,\mathrm{L})\,ij}_{\mathbf{v}_\beta,n;\,\mathbf{v}_\beta,\,f_\beta} \\
&\quad + C^{(1\,e\,\mathrm{C})\,ik}_{\mathbf{v}_\alpha,m;\,f_\alpha}\,\chi_{f_\alpha}(\mathbf{r}_1)\left[\partial^k\partial^j\,g(\mathbf{r}_1-\mathbf{r}_2)\right]\chi_{t_\beta}(\mathbf{r}_2)\,C^{(2\,e\,\mathrm{C})\,ij}_{\mathbf{v}_\beta,n;\,t_\beta} \\
&\quad + C^{(1\,e\,\mathrm{C})\,ik}_{\mathbf{v}_\alpha,m;\,f_\alpha}\,\chi_{f_\alpha}(\mathbf{r}_1)\left[\partial^k\partial^j\,g(\mathbf{r}_1-\mathbf{r}_2)\right]\phi_{\mathbf{v}_\beta,\,f_\beta}(\mathbf{r}_2)\,C^{(2\,e\,\mathrm{L})\,ij}_{\mathbf{v}_\beta,n;\,\mathbf{v}_\beta,\,f_\beta} \Big\} \\
&\quad \equiv C^{(1\,e\,\mathrm{C})\,i}_{\mathbf{v}_\alpha,m;\,f_\alpha}\,C^{(2\,e\,\mathrm{C})\,ij}_{\mathbf{v}_\beta,n;\,t_\beta}\,A^j(f_\alpha;t_\beta) \\
&\quad + C^{(1\,e\,\mathrm{C})\,i}_{\mathbf{v}_\alpha,m;\,f_\alpha}\,C^{(2\,e\,\mathrm{L})\,ij}_{\mathbf{v}_\beta,n;\,\mathbf{v}_\beta,\,f_\beta}\,A^j(f_\alpha;\mathbf{v}_\beta,f_\beta) \\
&\quad + C^{(1\,e\,\mathrm{C})\,i}_{\mathbf{v}_\alpha,m;\,f_\alpha}\,C^{(2\,e\,\mathrm{C})\,ij}_{\mathbf{v}_\beta,n;\,t_\beta}\,A^j(f_\alpha;t_\beta) \\
&\quad + C^{(1\,e\,\mathrm{C})\,i}_{\mathbf{v}_\alpha,m;\,f_\alpha}\,C^{(2\,e\,\mathrm{L})\,ij}_{\mathbf{v}_\beta,n;\,\mathbf{v}_\beta,\,f_\beta}\,A^j(f_\alpha;\mathbf{v}_\beta,f_\beta) \\
&\quad + C^{(1\,e\,\mathrm{C})\,ik}_{\mathbf{v}_\alpha,m;\,f_\alpha}\,C^{(2\,e\,\mathrm{C})\,ij}_{\mathbf{v}_\beta,n;\,t_\beta}\,A^{kj}(f_\alpha;t_\beta) \\
&\quad + C^{(1\,e\,\mathrm{C})\,ik}_{\mathbf{v}_\alpha,m;\,f_\alpha}\,C^{(2\,e\,\mathrm{L})\,ij}_{\mathbf{v}_\beta,n;\,\mathbf{v}_\beta,\,f_\beta}\,A^{kj}(f_\alpha;\mathbf{v}_\beta,f_\beta) \\
&\quad \equiv C^{(1\,e\,\mathrm{C})\,i}_{\mathbf{v}_\alpha,m;\,f_\alpha}\,C^{(2\,e\,\mathrm{C})\,ij}_{\mathbf{v}_\beta,n;\,t_\beta}\,A^j(f_\alpha;t_\beta) \\
&\quad + C^{(1\,e\,\mathrm{C})\,i}_{\mathbf{v}_\alpha,m;\,f_\alpha}\,C^{(2\,e\,\mathrm{L})\,ij}_{\mathbf{v}_\beta,n;\,\mathbf{v}_\beta,\,f_\beta}\,A^j(f_\alpha;\mathbf{v}_\beta,f_\beta) \\
&\quad + C^{(1\,e\,\mathrm{C})\,i}_{\mathbf{v}_\alpha,m;\,f_\alpha}\,C^{(2\,e\,\mathrm{C})\,ij}_{\mathbf{v}_\beta,n;\,t_\beta}\,A^j(f_\alpha;t_\beta) \\
&\quad + C^{(1\,e\,\mathrm{C})\,i}_{\mathbf{v}_\alpha,m;\,f_\alpha}\,C^{(2\,e\,\mathrm{L})\,ij}_{\mathbf{v}_\beta,n;\,\mathbf{v}_\beta,\,f_\beta}\,A^j(f_\alpha;\mathbf{v}_\beta,f_\beta) \\
&\quad + C^{(1\,e\,\mathrm{Cn})\,i}_{\mathbf{v}_\alpha,m;\,f_\alpha}\,C^{(2\,e\,\mathrm{C})\,ij}_{\mathbf{v}_\beta,n;\,t_\beta}\,A^j_{\mathrm{n}}(f_\alpha;t_\beta) \\
&\quad + C^{(1\,e\,\mathrm{Cn})\,i}_{\mathbf{v}_\alpha,m;\,f_\alpha}\,C^{(2\,e\,\mathrm{L})\,ij}_{\mathbf{v}_\beta,n;\,\mathbf{v}_\beta,\,f_\beta}\,A^j_{\mathrm{n}}(f_\alpha;\mathbf{v}_\beta,f_\beta)\ .
\end{aligned}
\tag{6.86}
$$

The contribution $A^{(e)}$:

$$C^{(1\,f\,\mathrm{C})\,i}_{\mathbf{v}_\alpha,m;\,f_\alpha} = \left(\frac{\hat{\mathbf{n}}_{\mathbf{v}_\alpha,\,t_\alpha+}\cdot\hat{\mathbf{n}}_{f_\alpha}}{h_{\mathbf{v}_\alpha,\,t_\alpha+}} - \frac{\hat{\mathbf{n}}_{\mathbf{v}_\alpha,\,t_\alpha-}\cdot\hat{\mathbf{n}}_{f_\alpha}}{h_{\mathbf{v}_\alpha,\,t_\alpha-}}\right)\hat{n}^m_{f_\alpha}\,\hat{n}^i_{f_\alpha}\ , \quad f_\alpha \in \mathcal{F}_\alpha\ , \tag{6.87a}$$

$$C^{(1\,f\,\mathrm{B})\,i}_{\mathbf{v}_\alpha,m;\,f_\alpha} = \frac{1}{h_{\mathbf{v}_\alpha,\,t_\alpha}}\,\hat{n}^m_{f_\alpha}\,\hat{n}^i_{f_\alpha}\ , \quad f_\alpha \in \partial\mathcal{T}_\alpha\ , \tag{6.87b}$$

$$C^{(1\,f\,\mathrm{B})\,ij}_{\mathbf{v}_\alpha,m;\,f_\alpha} = \frac{1}{h_{\mathbf{v}_\alpha,\,t_\alpha}}\,\hat{n}^m_{f_\alpha}\,\hat{n}^i_{f_\alpha}\,\hat{n}^j_{f_\alpha}\ , \quad f_\alpha \in \partial\mathcal{T}_\alpha\cap\partial\Omega\ , \tag{6.87c}$$

$$C^{(1\,f\,\mathrm{Bn})\,i}_{\mathbf{v}_\alpha,m;\,f_\alpha} = \frac{1}{h_{\mathbf{v}_\alpha,\,t_\alpha}}\,\hat{n}^m_{f_\alpha}\,\hat{n}^i_{f_\alpha}\ , \quad f_\alpha \in \partial\mathcal{T}_\alpha\cap\partial\Omega\ , \tag{6.87d}$$

$$\begin{aligned} C^{(2\,f\,\mathrm{C})\,i}_{\mathbf{v}_\beta,n;\,t_\beta} = {} & \left(\frac{\rho_0}{\rho(f_\beta+)} - \frac{\rho_0}{\rho(f_\beta-)}\right)\frac{\rho(t_\beta)}{\rho_0}\,X_{iknl}(t_\beta) \\ & \frac{1}{h_{\mathbf{v}_\beta,\,t_\beta}}\,\hat{n}^k_{f_\beta,\,t_\beta}\,\hat{n}^l_{\mathbf{v}_\beta,\,t_\beta}\ , \quad t_\beta \in \mathcal{T}_\beta\ , \quad f_\beta \in \partial t_\beta\ . \end{aligned} \tag{6.87e}$$

In terms of these coefficients, the matrix element (6.82), written in the form of Eq.(6.84), is

$$\begin{aligned} A^{(e)}_{\mathbf{v}_\alpha,m;\mathbf{v}_\beta,n} = {} & \sum_{\nu_1\,\nu_2} B^{(dXX)}(\nu_1,\nu_2)\int \mathrm{d}r_1 \int \mathrm{d}r_2 \\ & C^{(1\,f\,\nu_1)\,I_1}_{\mathbf{v}_\alpha,m;\,M_1}\,\phi_{M_1}(\mathbf{r}_1)\left[\mathcal{D}^{I_1\,I_2}\,g(\mathbf{r}_1-\mathbf{r}_2)\right]\phi_{M_2}(\mathbf{r}_2)\,C^{(2\,f\,\nu_2)\,I_2}_{\mathbf{v}_\beta,n;\,M_2} \\ = {} & \int \mathrm{d}r_1 \int \mathrm{d}r_2 \\ & \Big\{ C^{(1\,f\,\mathrm{C})\,i}_{\mathbf{v}_\alpha,m;\,f_\alpha}\,\chi_{f_\alpha}(\mathbf{r}_1)\,g(\mathbf{r}_1-\mathbf{r}_2)\,\chi_{f_\beta}(\mathbf{r}_2)\,C^{(2\,f\,\mathrm{C})\,i}_{\mathbf{v}_\beta,n;\,f_\beta} \\ & + C^{(1\,f\,\mathrm{B})\,i}_{\mathbf{v}_\alpha,m;\,f_\alpha}\,\chi_{f_\alpha}(\mathbf{r}_1)\,g(\mathbf{r}_1-\mathbf{r}_2)\,\chi_{f_\beta}(\mathbf{r}_2)\,C^{(2\,f\,\mathrm{C})\,i}_{\mathbf{v}_\beta,n;\,f_\beta} \\ & + C^{(1\,f\,\mathrm{B})\,ij}_{\mathbf{v}_\alpha,m;\,f_\alpha}\,\chi_{f_\alpha}(\mathbf{r}_1)\left[\partial^j\,g(\mathbf{r}_1-\mathbf{r}_2)\right]\chi_{f_\beta}(\mathbf{r}_2)\,C^{(2\,f\,\mathrm{C})\,i}_{\mathbf{v}_\beta,n;\,f_\beta}\Big\} \\ \equiv {} & C^{(1\,f\,\mathrm{C})\,i}_{\mathbf{v}_\alpha,m;\,f_\alpha}\,C^{(2\,f\,\mathrm{C})\,i}_{\mathbf{v}_\beta,n;\,f_\beta}\,A(f_\alpha;f_\beta) \\ & + C^{(1\,f\,\mathrm{B})\,i}_{\mathbf{v}_\alpha,m;\,f_\alpha}\,C^{(2\,f\,\mathrm{C})\,i}_{\mathbf{v}_\beta,n;\,f_\beta}\,A(f_\alpha;f_\beta) \\ & + C^{(1\,f\,\mathrm{B})\,ij}_{\mathbf{v}_\alpha,m;\,f_\alpha}\,C^{(2\,f\,\mathrm{C})\,i}_{\mathbf{v}_\beta,n;\,f_\beta}\,A^j(f_\alpha;f_\beta) \\ \equiv {} & C^{(1\,f\,\mathrm{C})\,i}_{\mathbf{v}_\alpha,m;\,f_\alpha}\,C^{(2\,f\,\mathrm{C})\,i}_{\mathbf{v}_\beta,n;\,f_\beta}\,A(f_\alpha;f_\beta) \\ & + C^{(1\,f\,\mathrm{B})\,i}_{\mathbf{v}_\alpha,m;\,f_\alpha}\,C^{(2\,f\,\mathrm{C})\,i}_{\mathbf{v}_\beta,n;\,f_\beta}\,A(f_\alpha;f_\beta) \\ & + C^{(1\,f\,\mathrm{Bn})\,i}_{\mathbf{v}_\alpha,m;\,f_\alpha}\,C^{(2\,f\,\mathrm{C})\,i}_{\mathbf{v}_\beta,n;\,f_\beta}\,A_{\mathrm{n}}(f_\alpha;f_\beta)\ . \end{aligned} \tag{6.88}$$

6.5 Tetrahedron-tetrahedron contributions to stiffness matrix elements

Each of the matrix elements for "composite" basis functions is, generally, a sum of many contributions of pairs of "fundamental" basis function. This is, in particular, the case for node based functions, where a vertex may be shared by many tetrahedra and facets.

We now estimate the number of contributing tetrahedra and facets, e.g., the number of t_α, f_α, etc., entries in each "row" of the coefficient matrices of Eqs. (6.85) and (6.87). We are considering here the generic case of a vertex located in the interior of a regular tetrahedral mesh (approximately constant edge lengths).

First, we note that the number of tetrahedra t_α in the set $\mathcal{T}_\alpha$, or, equivalently, the number of facets f_α in the set $\partial\mathcal{T}_\alpha$, is approximately equal to the number of triangles in a regular triangulation of the unit sphere. Since the area of a triangle is $A \simeq \sqrt{3}/4$, the number of such triangles covering the sphere is about $4\pi/A \simeq 4\pi/(\sqrt{3}/4) = 16\,\pi/\sqrt{3}$. Secondly, the number of facets f_α sharing the given vertex, i.e., the number of elements in the set $\mathcal{F}_\alpha$, is equal to the number of edges in the considered triangulation of the sphere, which is about 3/2 the number of facets, hence $(3/2)\,16\,\pi/\sqrt{3} = 8\sqrt{3}\,\pi$. Hence,

$$\#\mathcal{T}_\alpha = \#\partial\mathcal{T}_\alpha \simeq \frac{16\,\pi}{\sqrt{3}} \simeq 29.0 \tag{6.89a}$$

and

$$\#\mathcal{F}_\alpha \simeq 8\sqrt{3}\,\pi \simeq 43.5\ . \tag{6.89b}$$

6.6 Construction of the stiffness matrix

In designing the solver code, we have to allow sufficient flexibility in order to accommodate various types of equations, various sets of unknowns, and expressions for matrix elements.

General structure of matrix elements. All the expressions for the matrix elements involving the Green function,[3] i.e., Eqs. (6.81), (6.82), and (6.39) – (6.43) have the structure indicated in Eq.(6.84). More explicitly, for a given equation type, a matrix block corresponding to two fixed types of unknowns[4] has the form

$$A_{\alpha\beta} = \sum_{\nu_1\,\nu_2} B(\nu_1,\nu_2) \sum_{g_1,\,b_1} \sum_{g_2,\,b_2} \sum_{\ell} C^{(1\,\nu_1)\,I_1(\ell)}_{\alpha;\,g_1,b_1}\, C^{(2\,\nu_2)\,I_2(\ell)}_{\beta;\,g_2,b_2}\, A^{(M(\nu_1,\nu_2))\,I(\ell)}(g_1,b_1;g_2,b_2)\ . \tag{6.90}$$

The notation here is as follows:

1. Within the considered block, unknowns are labeled locally by integer indices α, β.

2. The sets of coefficients C are stored as arrays indexed by the indices ν_j, $j = 1,2$; the order of the entries in the array is arbitrary.

3. Similarly, the "basic" matrix elements $A^{(\nu)\,I}(\cdot)$ are labeled by an index ν, which defines the type of the matrix element (e.g., between a linear function on a tetrahedron and a constant function on a facet, and with the normal derivative of the Green function). Actually, in the actual code implementation the matrix elements A are not stored, but rather computed as needed (in a loop which ensures there no replication of work); in this case the index ν is an argument of the routine computing the matrix elements and specifies which element is to be evaluated.

[3]The matrix elements given by single integrals, as well as projections of the incident or scattered waves on the basis function, can be treated as special cases.

[4]E.g., the row indices α may refer to displacement, and the column indices β to pressure.

4. The indices ν_j, $j = 1, 2$, refer to consecutive sets of the coefficients C; they form an array of coefficient sets, and may be ordered in an arbitrary way.

5. Accordingly, the coefficients $B(\nu_1, \nu_2)$ define weights with which pairs of coefficients C contribute to the sum.

6. Similarly, the integer indices $M(\nu_1, \nu_2)$ specify which type of a matrix element is to be used with the given coefficients C.

7. The indices g_1 and g_2 refer to g-element types (in the present problems, tetrahedra or triangles), and the indices b_1 and b_2 to consecutive numbers of basis functions associated with a given g-element; e.g., if the considered basis functions are linear and the g-element is a tetrahedron, the index b may take values from 1 to 4, and indicate the tetrahedron vertex at which the basis function value is 1.

8. The coefficients $C^{(j\,\nu_j)\,I_j}_{\alpha,\,g_j,\,b_j}$ provide relations between the unknowns and the basis functions; they depend, in general, on the material properties of the object.

9. The quantities $A^{(\nu)\,I}(g_1,\, b_1; g_2,\, b_2)$ are the "basic" matrix elements, such as listed in Section 6.3.5. As we mentioned before, the index ν may be used to specify various types of matrix elements.

10. The integer indices I_j in the coefficients $C^{(j\,\nu_j)\,I_j}_{\alpha,\,g_j,\,b_j}$ specify vector or tensor indices. If C is a rank-1 tensor and is labeled by a single index, I_j may be identified with that index. If C is a rank-2 tensor, then the index I_j may refer to pairs of Cartesian indices; for example, if the tensor is symmetric,[5] the consecutive values $1, 2, \ldots, 6$ of I_j may correspond to pairs $(1,1), (1,2), \ldots, (3,3)$.

11. The indices I in the matrix elements $A^{(\nu)\,I}(\cdot)$ have the same meaning as in the coefficients C. (In practice, I will be usually just a single Cartesian index.)

12. The tensor algebra (index contraction) is handled by taking the sum over ℓ: the arrays $I_j(\ell)$ and $I(\ell)$ define then the matching tensor indices, their pairs, etc.

Matrix storage. In practice, for larger problems it is always necessary to use matrix compression. Hence, the matrix blocks $A^{\nu_1\,\nu_2}$ are stored as sparse matrices, involving only couplings between spatially close geometry elements. Therefore, an important aspect of matrix construction is determination of its sparsity structure, based on distances between the geometry elements; the problem is relatively complex, since different near-field ranges will be needed for various types of matrix elements (near-field matrix element computation and storage is expensive, hence we want to reduce the near field range as much as possible). In addition, of course, we will have to store additional matrix data required in compression, such as coefficients for mapping basis functions into equivalent Cartesian-grid sources.

Further, parallel implementation of the solver requires utilization of geometry segments (slices or stacks of slices) rather than a single global geometry. Thus, matrix blocks are always constructed, on a given processor, by using locally available geometry segments.

[5]The symmetry may follow, e.g., from the relations (6.66).

Organizing matrix construction. Obviously, the most time consuming element in the matrix computation is the evaluation of the basic matrix elements $A(g_1, b_1; g_2, b_2)$ themselves. Therefore, in order to minimize the computational cost without introducing additional storage, many (perhaps all) matrix blocks should be created incrementally, but in parallel – in the sense that, having computed a given matrix element $A(g_1, b_1; g_2, b_2)$, one should add its contribution to all relevant matrix elements. One sould also carry out far-field subtractions on-the-fly, while storing near-field matrix elements (this is particularly important in the parallel computation).

The envisaged scheme is as follows

1. Compute blocks of coefficients $C^{(j\,\nu_j)}$.

2. Compute MoM-Cartesian mappings.

3. Compute maps D "inverse" to the maps C, in the sense of mapping a given geometry element onto a set of unknowns. We define separate maps D for the types of geometry elements involved (here, tetrahedra and facets) and for the types of unknowns (e.g., pressure and displacement). I.e., for each type of the g-element g and each type of unknown ν we define a matrix $D^{(j\,\nu_j)}_{g;\alpha}$, in integer compressed sparse row format (integer CSR); rows of this matrix will be labeled by the g-elements and each row will contain a list of unknown numbers corresponding to the basis function numbers b.

4. Compute sparsity patterns of matrix blocks (or "sub-blocks", if various types of elements are involved – e.g., interface and interior elements, etc.). In the parallel code, the computed sparsity patterns must take into account location of elements in geometry segments; e.g., row indices must always refer to the "home" geometry slice, while column indices may refer to elements in the stack of slices.

5. On the basis of nonzero coefficients $C^{(j\,\nu_j)}$ and the sparsity patterns, create lists of geometry elements that will be required in the matrix computation (or, maybe, set flags for elements in the input geometries). For instance, we may use all tetrahedra in the geometry, but only some triangles (those at interfaces), etc.

6. Carry out loops over selected geometry elements. For each pair of elements:

   (a) compute all basic matrix elements (as required by the coefficients $C^{(j\,\nu_j)}$ and sparsity patterns);

   (b) compute far-field subtractions (in terms of the MoM-Cartesian mappings) and modify the evaluated matrix elements;

   (c) add their contributions to the required blocks.

   Schematically, if we assume the sparsity patterns are stored in terms of g-elements, the structure of the loop is

for $\texttt{ng1} = 1, \ldots, \texttt{nng1}$
// get geometry data γ_1 of g-element $\texttt{ng1}$
// compute and store MoM-Cartesian mapping coefficients for g-elem. $\texttt{ng1}$:
$W_1 = W^{(1)}(\gamma_1)$
// get number of near elements in the sparsity pattern:
$\texttt{nng2} = \ldots$
for $\texttt{ng2} = 1, \ldots, \texttt{nng2}$
// get geometry data γ_2 of g-element $\texttt{ng2}$
// compute MoM-Cartesian mapping coefficients for g-elem. $\texttt{ng2}$:
$W_2 = W^{(2)}(\gamma_2)$
// store W_2 only for γ_2 in home slice
// get basic MoM matrix element for the g-elements γ_1, γ_2:
$A^{\mathrm{MoM}} = A(\gamma_1, \gamma_2)$
// get basic far-field matrix element for the g-elements γ_1, γ_2:
// [this should be modified to take into account derivatives of g]
$A^{\mathrm{Far}} = W_1\, g\, W_2^{\mathrm{T}}$
// get numbers of unknowns associated with γ_1 and γ_2:
$\texttt{kkx1} = K(D^{(1)}(\texttt{ng1}))$ (6.91)
$\texttt{kkx2} = K(D^{(2)}(\texttt{ng2}))$
for $\texttt{kx1} = 1, \ldots, \texttt{kkx1}$
// get unknown number from inverse mapping:
$\texttt{nx1} = D^{(1)}(\texttt{ng1}, \texttt{kx1})$
// get the coefficient relating the unkn. $\texttt{nx1}$ and the g-elem. $\texttt{ng1}$:
$c_1 = C^{(1)}(\texttt{nx1}, \texttt{ng1})$
for $\texttt{kx2} = 1, \ldots, \texttt{kkx2}$
// get unknown number from inverse mapping:
$\texttt{nx2} = D^{(2)}(\texttt{ng2}, \texttt{kx2})$
// get the coefficient relating the unkn. $\texttt{nx2}$ and the g-elem. $\texttt{ng2}$:
$c_2 = C^{(2)}(\texttt{nx2}, \texttt{ng2})$
// add computed contribution to the output matrix element:
$A(\texttt{nx1}, \texttt{nx2}) \mathrel{+}= c_1\, c_2\, (A^{\mathrm{MoM}} - A^{\mathrm{Far}})$
endfor $\texttt{kx2}$
endfor $\texttt{kx1}$
endfor $\texttt{ng2}$
endfor $\texttt{ng1}$

We stress that in the above scheme the MoM-Cartesian mapping is computed on-the-fly. Out of all the mapping coefficient sets W we store only those which are needed in the

matrix-vector multiplication.

7 Implementation of the volumentric integral-equations code for elasticity

We describe here the initiated implementation of the integral solver code for elasticity. The work is in progress, and its main goal is to develop a comprehensive library of functions covering various types of integral equations described in this report.

7.1 The code structure

The present version of the code contains several routines written to allow testing of various types of integral equations in acoustics.

The general idea of the code is to use combinations of as simple routines as possible. In particular, geometry data, mapping between geometry elements and unknowns, and material data are kept separate, and handled, as far as possible, by separate routines. Thus, for example, there are separate routines for

1. Computing mapping between geometry elements ("g-elements") and unknowns, using as input geometry and material data.

2. Generating sparsity pattern of the near-field matrix blocks, using as input geometry, geometry-unknown mapping, and compression data.

3. Generating sparsity pattern of the near-field matrix blocks, using as input geometry, geometry-unknown mapping, and compression data.

4. Generating blocks of "basic" matrix elements between the "fundamental" basis functions supported on g-elements, using as input geometry, geometry-unknown mapping, and matrix sparsity patterns.

5. Generating sets of material-depending coefficients appearing in matrix elements for the actual equations (defined in terms of the "composite" basis functions).

6. Assembling matrix blocks of the final matrix for the given integral equation, using as input geometry (its connectivity data), matrix blocks for the "fundamental" basis functions, and the material-dependent coefficients computed in the previous step.

7. Generating MoM-to-Cartesian mapping coefficients for the "fundamental" basis functions, using as input geometry and geometry-unknown mapping.

8. Assembling MoM-to-Cartesian mapping coefficients for the "composite" basis functions, using as input geometry, the previously computed mapping, and the material-dependent coefficients.

Blocks of the MoM matrix are computed according to the formula

$$
\begin{aligned}
& A^{(\nu)}_{\alpha_1=K_1(\nu,\kappa)\,\rho_1(\nu,\kappa,r_1)+I_1(\nu,\kappa,t)\,,\;\alpha_2=K_2(\nu,\kappa)\,\rho_2(\nu,\kappa,r_2)+I_2(\nu,\kappa,t)} \\
& \quad += \sum_{\sigma_1}\sum_{\sigma_2}\sum_{\gamma_1}\sum_{\gamma_2}\sum_{\nu=1}^{\nu_{\max}}\sum_{\kappa=1}^{K_\nu} B^{(\nu)}_{\kappa}\sum_{r_1}\sum_{r_2}\sum_{t=1}^{t_\kappa} \\
& \qquad C^{(1)}(\nu,\kappa,r_1,I_1(\nu,\kappa,t))\,C^{(2)}(\nu,\kappa,r_2,I_2(\nu,\kappa,t))\,A^{(\nu,\,\kappa,\,I(\nu,\kappa,t))}_{\sigma_1\gamma_1\,,\,\sigma_2\gamma_2}\ ,
\end{aligned}
\tag{7.1}
$$

which is more explicit from of Eq.(6.90).

The expression (7.1) represents a set of $\nu_{\max}$ matrix blocks, $\nu = 1, \ldots, \nu_{\max}$. The ν sum on its r.h.s. has to be understood as a loop in which contributions to the individual matrix blocks are being accumulated. In this loop the unknown numbers α_1 and α_2 are expressed in terms of the tensor indices I_1 and I_2, which are given by the tensor multiplication table for the given matrix block number ν and the given pair κ of mapping data. The tensor index I – selecting an element from the set of the basic matrix elements – is also determined by the tensor multiplication table. The unknowns indices α_1 and α_2, labeling the output matrix element, are functions of the sum (loop) indices ν, κ, r_1, r_2, and t.

The actual implementation of the expression (7.1), in terms of loops and variables in the code, is given by Eq.(7.18). To facilitate the comparison of the formula (7.1) and the pseudo-code, we show here the correspondence between the relevant quantities, particularly

the indices (labeled by $j = 1, 2$):

$$
\begin{aligned}
\nu_{\max} &\to \texttt{nnu} && \text{(number of matrix blocks)}\ , \\
\sigma_j &\to \texttt{kgt}j && (\textbf{g-element type})\ , \\
\gamma_j &\to \texttt{ng}j && (\textbf{g-element number})\ , \\
\nu &\to \texttt{nu} && (\textbf{matrix block number})\ , \\
K_\nu &\to \texttt{kkcc} && \\
&\quad \texttt{= ppcb[nu]->pcob->na} && \text{(number of pairs of mapping data sets)}\ , \\
\kappa &\to \texttt{kcc} && (\textbf{index of a pair of mapping data sets})\ , \\
B_\kappa^{(\nu)} &\to \texttt{cb} && \\
&\quad \texttt{= ppcb[nu]->pcob->paa[kcc]} && \text{(value of the coupling coefficient)}\ , \\
c_1 &\to \texttt{nca}j && \\
&\quad \texttt{= ppcb[nu]->pcob->pia[kcc]} && \text{(index of the first mapping data set)}\ , \\
c_2 &\to \texttt{nca}j && \\
&\quad \texttt{= ppcb[nu]->pcob->pja[kcc]} && \text{(index of the second mapping data set)}\ , \\
K_j &\to \texttt{kkxc}j && \\
&\quad \texttt{= ppca}j\texttt{[nca}j\texttt{]->kkx} && \text{(number of unknowns per reduced unkn.)}\ , \\
r_j &\to \texttt{nar}j && (\textbf{g-element} \to \textbf{unkn. mapping index})\ , \\
\rho_j &\to \texttt{nr}j && \\
&\quad \texttt{= ppca}j\texttt{[nca}j\texttt{]->pcsr->pja[nar}j\texttt{]} && \text{(reduced unknown index)}\ , \\
t &\to \texttt{nat} && (\textbf{number of tensor multipl. table})\ , \\
I_1 &\to \texttt{ni1} && \\
&\quad \texttt{= ppcb[nu]->ppcot[kkc]->pia[nat]} && \text{(first tensor index)}\ , \\
I_2 &\to \texttt{ni2} && \\
&\quad \texttt{= ppcb[nu]->ppcot[kkc]->pja[nat]} && \text{(second tensor index)}\ , \\
I &\to \texttt{nia} && \\
&\quad \texttt{= ppcb[nu]->ppcot[kkc]->paa[nat]} && \text{(tensor index of the basic matrix element)}\ , \\
\alpha_j &\to \texttt{nx}j && \\
&\quad \texttt{= kkxc}j\texttt{ * nr}j\texttt{ + ni}j && \text{(unknown number)}\ .
\end{aligned}
\tag{7.2}
$$

Running summation (loop) indices are marked with boldface descriptions.

The main point of using the scheme of computation of Eq.(7.1) and the code (7.18) is to minimize the amount of work and storage in the most expensive operations of computing the “basic” matrix elements (between the “elementary” basis functions). A set of such elements, with all required tensor indices I, is evaluated for the given pair of g-elements, γ_1 and γ_1, as soon as these indices are set, i.e., ***outside*** the sums/loops over the indices ν, κ, r_1, and r_2. This set of values is only stored temporarily, and its contributions to all blocks and elements of the matrix are evaluated in the inner loops (through ν, κ, r_1, r_2).

The procedure of generating input data for the computation of the stiffness matrix blocks, and the actual computation is shown, schematically, in Fig. 3. We will repeatedly refer to this Figure and explain its details in the following.

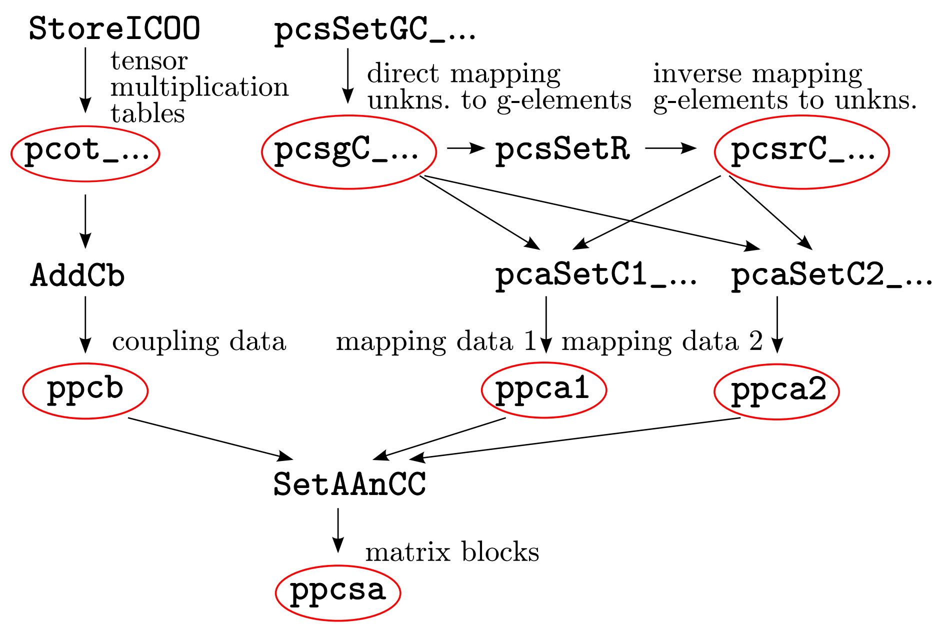

Figure 3: Schematics of construction of matrix blocks. Data are marked with ovals, the remaining entries are routines called in the code.

7.2 Data structures

Geometry elements, basis functions, and unknowns. As an input to construction of the stiffness matrix, we consider two types of geometries:

1. Two-dimensional manifolds discretized with triangles. The triangles (or ***facets***, denoted by f) are referred to as ***s-elements*** (surface elements) and the edges as the as ***b-elements*** (boundary elements). Those geometries form boundaries of and interfaces separating various material regions.

2. Three-dimensional manifolds discretized with tetrahedra (a generalization to hexahedra is possible but only partly implemented). In this case the tetrahedra (denoted by t) are referred to as ***s-elements*** and the their boundaries (i.e., triangular facets, denoted by f) as ***b-elements***.

Hence,

2-dim:	s-element: facet f	b-element: edge e ,	(7.3a)
3-dim:	s-element: tetrahedron t	b-element: facet f .	(7.3b)

We refer to all these geometry elements as "g-elements". The elements are oriented, i.e., an edge are defined as an ordered pair of vertices, and a facet as an ordered triplet, defining the direction of the normal according to the right-handed screw rule.

In the code s-elements are usually indexed by `ns` and b-elements by `nb`. The index `ng` is normally used for general g-elements.

Geometries are described in the code by the structure `CGEO`, whose main elements are:

1. `cdim`: number of dimensions of the geometry (as a manifold), i.e., 1 for a curve, 2 for a surface, 3 for a volume.

2. `nnv`: number of vertices.

3. `nns`: number of s-elements.

4. `nnb`: number of b-elements.

5. `nsvx`: number of vertices per s-element, e.g., 4 for tetrahedra.

6. `nbvx`: number of vertices per b-element, e.g., 3 for triangles (facets).

7. `nnsd`: number of sides of an s-element, e.g., 4 for tetrahedra.

8. `pvx`: array of sequentially stored (x, y, z) coordinates of the vertices, hence `3 * nnv` floating point numbers.

9. `psv`: array of numbers of vertices defining s-elements, hence `nsvx * nns` integers, with values from 1.

10. `pbv`: array of numbers of vertices defining b-elements, hence `nbvx * nnb` integers, with values from 1.

11. `psb`: array of numbers of b-elements forming boundaries of s-elements, hence `nnsd * nns` integers, with signed values from ± 1. The signs define orientation of a b-element with respect to the s-element. E.g., for `cdim` $= 3$, `psb` > 0 if the facet (b-element) orientation is away from the tetrahedron (s-element). Similarly, for `cdim` $= 2$, `psb` > 0 if the edge (b-element) orientation relative to the facet (s-element) is counter-clockwise (looking from the positive side of the facet).

12. `pbs`: array of numbers of s-elements adjacent to b-elements, hence `2 * nnb` integers, with values from 1. The first entry in each pair is the number of the s-element on the negative side of the b-element. If the b-element is a facet, its negative side is opposite the direction of the normal. If it is an edge, its negative side is the left side when looking from the positive side of the surface. If the b-element has only one adjacent s-element, the missing entry in the pair is zero.

We also consider several types of "fundamental" basis functions associated with s-elements of the geometry:

(i) For `cdim` $= 2$:

1. Constant scalar basis functions supported on facets.
2. Linear scalar basis functions supported on facets.
3. Linear vector basis functions supported on facets.

(ii) For cdim $= 3$:

1. Constant scalar basis functions supported on tetrahedra.
2. Linear scalar basis functions supported on tetrahedra.
3. Linear vector basis functions supported on tetrahedra.

The above basis functions can be combined to form "composite" basis functions supported on sets of s-elements, and associated with various g-elements. There are also relations between some of these basis functions and derivatives of other functions.

Material parameters. We assume material parameters constant over s-elements. In the code they are described by the pair (kkms, pms), where int kkms is the number of parameters per s-element, and COMPLEX pms[] is the array of parameter values stored sequentially for all s-elements (i.e., kkms * nns complex numbers). For example, in acoustics we have kkms $= 2$, corresponding, e.g., to relative density and relative compressibility of the material. In elasticity we need kkms $= 3$ in order to access relative density, and relative values of Lamé coefficients.

Tensor tables. The tables used to combine tensor indices of basis functions into indices of matrix elements are stored in predefined integer matrices in the coordinate format, MI_COO *pcot. They appear in Fig. 3 under the generic name pcot_.... A set of various tables is defined and then used as input to further operations.

Unknown ↔ g-element mapping tables. These tables are stored as integer matrices in the sparse-row format, MI_CSR *pcsg (for the "forward" mapping from unknowns to g-elements) and MI_CSR *pcsr (for the inverse mapping). More details on these mappings are given below in the description of the structure CCFA of the mapping coefficients.

Unknown ↔ g-element mapping data. Sets of tables coefficients relating basis functions to g-elements (such as ppca1 and ppca2 in Fig. 3) are stored in structures CCFA defined in the header vmax_ccfa.h as

```
/* structure for storing C coefficients -- prefix ca */
typedef struct
{
  char          name[80];   /* name to identify the object */
  int           kxt[3];     /* unknown type:
                               kxt[0] -- unknowns associated with:
                               0(vertex) 1(edge) 2(facet) 3(tetrahedron)
                               kxt[1] -- physical quantity (tensor rank)
                               0(pressure) 1(displacement) 3(stress tensor)
                               kxt[2] -- physical problem type
                             */
  int           kgt;        /* g-element type:
                               0(vertex) 1(edge) 2(facet) 3(tetrahedron) */
  int           kbt;        /* basis function type: 0(const) 1(linear) */
  int           nnx;        /* number of unknowns */
  int           nnr;        /* reduced number of unknowns */
  int           kkx;        /* number of unknowns per "reduced unknown" */
  int           nni;        /* additional number of tensor components (not used) */
  /* mapping: unknowns --> geometry elements
     -- allocation: nnr (if nnr > 0) or nnx */
  MI_CSR        *pcsg;      /* arrays of lists of g-elements for (red.) unkns.
                             * row # (from 0) = nr = reduced unknown #
                             * col # (from 1) = ng = g-element #
                             * value (from 1) = kb = # of the basis fn. (< kkx)
                             */
  /* inverse mapping: geometry elements --> unknowns
     -- allocation: nng
     constructed as transpose of pcsg, except that the values
     are addresses nag in pcsg */
  MI_CSR        *pcsr;      /* arrays of lists of (red.) unknowns for g-elems.
                             * row # (from 0) = ng  = g-element #
                             * col # (from 1) = nr  = reduced unknown #
                             * value (from 1) = nag = storage # in pcsg
                             */
  /* coefficient values: */
  COMPLEX       *pgc;       /* array of values with access given by pcsg:
                               C = pgc[nag][kx][ni]
                               for each element of pcsg: [kkx][nni] values
                               (nni not used) */
} CCFA;
```

(7.4)

In this structure:

1. The array is given a name `name` for identification.
2. The array of three integers `kxt[3]` characterize the unknown type: the g-element with which the unknown is associated and the tensor rank related to the given physical quantity; the third number is currently not used (it is set to an undefined value, `-1`).

3. The integer kgt defines the g-element type.

4. The integer kgt defines the basis function type.

5. The integer nnx denotes the number of unknowns.

6. The integer nnr denotes the "reduced number of unknowns", i.e., generally, the number of unknowns not counting the number of their tensor components. E.g., for vector displacement unknowns nnr is equal to the number of vertices, while nnx is three times that number. By using nnr instead of nnx we can avoid replicating identical coefficients for several tensor components.

7. The related entry, kkx, is the number of unknowns per reduced unknown, e.g., 3 for a vector displacement unknown.

8. The entry nni is the number of tensor components characterizing the basis function.

9. The integer sparse-row format matrix MI_CSR *pcsg defines the mapping from reduced unknowns to geometry elements: its rows are indexed by reduced unknown numbers, columns by g-element numbers, and the values store the numbers of basis functions (up to kkx). Usually, to one unknown there correspond several g-elements; e.g., a vector displacement unknown associated with a vertex is supported by a set of tetrahedra sharing that vertex.

10. The integer sparse-row format matrix MI_CSR *pcsr defines the mapping inverse to the previous one, i.e., from geometry elements to the reduced unknowns: its rows are indexed by g-element numbers, and columns by reduced unknown numbers. In this case the values stored in the the matrix are storage numbers of elements in the previous matrix, pcsg. This information is used in constructing matrix elements in a loop through g-elements in the routine SetAAnCC, as described below.

11. Finally, the coefficient values are stored in the complex array pgc. The array contains kkx * nni values for each element of the mapping array pcsg. These values may, in general, depend on the material parameters.

Tables of coupling coefficients. Each MoM matrix block[6] is constructed by specifying a set of "coupling coefficients" which specify how to combine products of basis functions (associated with unknowns) into matrix elements. These coefficients are stored in a structure

[6]Compressed matrix blocks will be created in a similar scheme.

```
/* structure for storing coefficients B and multiplication tables T
   -- prefix cb */
typedef struct
{
  char          name[80];   /* name to identify the object (matrix block) */
  MC_COO        *pcob;      /* array of coefficients B defining couplings
                             * row # (from 0) = nu1 = number of the set C^1
                             * col # (from 1) = nu2 = number of the set C^2
                             * value          = b   = complex value of the coeff.
                             * elements are assumed to be sorted by rows and cols
                             */
  MI_COO        **ppcot;    /* array of index (tensor) multiplication tables
                             * one MI_COO matrix for each element of pcob
                             */
  TNAME         *ptname;    /* array of names of multiplication tables
                             * one name for each element of pcob
                             */
} CBFA;
```

(7.5)

In this structure:

1. The name `name` identifies the set of coupling coefficients and thus the resulting matrix block.
2. The complex coordinate-format matrix `MC_COO *pcob` specifies a set of pairs of unknown $\leftrightarrow$ g-element mapping data $(C^{(1)}, C^{(2)})$, identified by their numbers, and complex coefficients with which contributions of those pairs are to be added to the result.
3. To each element of the matrix `MC_COO *pcob` there corresponds a pointer to a tensor multiplication table.
4. Names of the above multiplication tables are also stored in an array.

7.3 Operations

We describe here the main operations executed by the code in assembling blocks of MoM matrix elements, according to the procedure represented in Fig. 3.

Structure of the matrix construction "driver". We reproduce below parts of the present main program which serves as a driver for generating blocks of the MoM matrix. This code is a simple illustration of the data flow shown in Fig. 3.

```
// set up material data: kkms1, pms1, kkms2, pms2

// set up two tensor multiplication tables
MI_COO *pcot = NULL;
// s s -> s (scalar scalar -> scalar)
StoreICOO(pcot_sss, 1, 1, 1);
// v v -> t (vector vector -> symmetric_tensor)
StoreICOO(pcot_vvt, 1, 1, 1);  StoreICOO(pcot_vvt, 1, 2, 2);
StoreICOO(pcot_vvt, 1, 3, 3);
StoreICOO(pcot_vvt, 2, 2, 4);  StoreICOO(pcot_vvt, 2, 3, 5);
StoreICOO(pcot_vvt, 3, 3, 6);

// create nnu = 2 sets of coupling data ppcb[]
nnu = 2;
// first set
pcb = ppcb[0];
AddCb(pcb, 1, 1, COMPLEX(1.), pcot_sss, "t_sss");
AddCb(pcb, 2, 1, COMPLEX(2.), pcot_sss, "t_sss");
// second set
pcb = ppcb[1];
AddCb(pcb, 1, 1, COMPLEX(2.), pcot_vtv, "t_vtv");
AddCb(pcb, 2, 1, COMPLEX(1.), pcot_vtv, "t_vtv");

// set up 3 unknown - g-element mapping tables pcsg...
// and inverse mapping tables pcsr...
// for G1:
pcsgC_f_dTvD = pcsSetGC_f_dTvD(pcgeo1);
pcsrC_f_dTvD = pcsSetR(pcsgC_f_dTvD);
pcsgL_f_Fv = pcsSetGL_f_Fv(pcgeo1);
pcsrL_f_Fv = pcsSetR(pcsgL_f_Fv);
// for G2:
pcsgC_t_Tv = pcsSetGC_t_Tv(pcgeo2);
pcsrC_t_Tv = pcsSetR(pcsgC_t_Tv);

// create nnca1 = 2 sets of mapping data for G1, nnca2 = 1 sets for G2
nnca1 = 2; nnca2 = 1;
// create elements of arrays of mapping data
// for G1:
ppca1[0] = pcaSetC1_C_f(pcgeo1, kkms1, pms1,
                        pcsgC_f_dTvD, pcsrC_f_dTvD, "C_f");
ppca1[1] = pcaSetC1_L_f(pcgeo1, kkms1, pms1,
                        pcsgL_f_Fv, pcsrL_f_Fv, "L_f");
// for G2:
ppca2[0] = pcaSetC2_C_t(pcgeo2, kkms2, pms2,
                        pcsgC_t_Tv, pcsrC_t_Tv, "C_t");

// compute nnu = 2 matrix blocks ppcsAn[]
SetAAnCC(ak0, pcgeo1, pcgeo2, nnu, ppcb, nnca1, nnca2, ppca1, ppca2, &ppcsAn);
```
(7.6)

Construction of tensor multiplication tables. In the initial stage of code execution we define a set of tables for operations on tensor indices of the basis functions and matrix elements. They are generated "by hand" by calling the routine StoreICOO (Fig. 3) and specifying nonzero elements of the tables. E.g., the table specifying a symmetric tensor in terms of two vectors is constructed by

```
// v v -> t (vector vector -> symmetric_tensor)
pcot = pcoICOOz();
StoreICOO(pcot, 1, 1, 1);
StoreICOO(pcot, 2, 2, 4);
StoreICOO(pcot, 2, 3, 5);
StoreICOO(pcot, 1, 2, 2);
StoreICOO(pcot, 1, 3, 3);
StoreICOO(pcot, 3, 3, 6);
MI_COO *pcot_vvt = pcoSortICOO(pcot);
```
(7.7)

These instructions (in which table elements may be entered in any order – they are sorted in the result) create a table named pcot_vvt which is shown in the test output as

```
T_vvt:

       1  2  3
--------------
    1  1  2  3
    2     4  5
    3        6
```
(7.8)

It indicates how the pairs of components of two vectors are assigned to the six independent components of the symmetric tensor; the row numbers refer to the first, and the column numbers to the second vector.

Construction of mapping tables. The code constructs a set of tables describing mapping between the unknowns and the g-elements (pcsgC_... and pcsgC_... in Fig. 3).

The forward mappings are generated, for specific cases, by separate routines, called with one of the geometries as the argument. For example, the forward mapping for linear basis functions supported on faces f in sets of faces $\mathcal{F}_{\mathbf{v}}$ sharing a vertex $\mathbf{v}$, in the first geometry, is generated by the routine

```
// Returns pcsg for linear b.f., f in F_v.
// input:
// pcgeo       = geometry
MI_CSR *pcsSetGL_f_Fv(CGEO *pcgeo)
```
(7.9)

in vmax_cffa_c.cpp. It is called as

```
MI_CSR *pcsgL_f_Fv = pcsSetGL_f_Fv(pcgeo1);
```
(7.10)

and stores the output as the array `pcsgL_f_Fv`.

All inverse mappings are generated from the forward ones by calling the same routine `pcsSetR`. E.g., in the considered example, the inverse mapping is obtained by

```
pcsrL_f_Fv = pcsSetR(pcsgL_f_Fv);                                    (7.11)
```

Construction of mapping data. The final set of mapping data, representing relations between the unknowns and g-elements (`ppca1` and `ppca2` in Fig. 3)

Specific tables of coefficients C for various sets of unknowns and basis functions are generated by specialized routines. For example, a set of coefficients $C^{(1)}$ for linear basis functions supported on faces is generated by the routine

```
// Computes and returns a set of C coefficients for a specific set
// of unknowns and basis functions
// input:
// pcgeo       = geometry
// kkms        = number of material parameters per s-element
// pms         = array of material parameters values for s-elements
// pcsg        = a mapping table: unknowns --> g-elements
// pcsr        = a mapping table: g-elements --> unknowns
// szName      = name of the set
//
// C for set 1 of linear basis functions supported on facets
CCFA *pcaSetC1_C_f(CGEO *pcgeo, int kkms, COMPLEX *pms,
                   MI_CSR *pcsg, MI_CSR *pcsr, char *szName)        (7.12)
```

It may be called with various unknown $\leftrightarrow$ g-element mappings. E.g., the call

```
pca1 = pcaSetC1_L_f(pcgeo1, kkms1, pms1,
                    pcsgL_f_Fv, pcsrL_f_Fv, "L_f");                  (7.13)
```

creates the coefficient set named `L_f` by using as arguments the geometry `pcgeo1`, material parameters specified by `kkms1` and `pms1`, and the mapping tables `pcsgL_f_Fv` and its inverse `pcsrL_f_Fv`. These mapping tables have been created previously (Eqs. (7.10) and (7.11)) for basis functions supported on faces f in sets of faces $\mathcal{F}_{\mathbf{v}}$ sharing a vertex $\mathbf{v}$.

One of the sets of the mapping data is shown in the test output as

```
C^(1)2:
----------------------
name:    L_f
kxt:     0     1    -1
kgt:     2
kbt:     1
nnx:         375
nnr:         125
kkx:           3
nni:           3
pcsg:
125 rows, 1020 columns, 3060 elements
rows: 1 ... 125 (125), columns: 1 ... 1020 (1020)
pcsr:
1020 rows, 125 columns, 3060 elements
rows: 1 ... 1020 (1020), columns: 1 ... 125 (125)
#g:         3060      #g / #r:     24.5
pgc:       27540 elements |C|:        13139.8
```
(7.14)

Construction of coupling data. The coupling data (an array of which is denoted by ppcb in Fig. 3) are constructed "by hand" by selecting specific sets of mapping data pairs $(C^{(1)}, C^{(2)})$, the corresponding coefficients, and the tensor multiplication tables. For instance, the second set of coupling data in the example code is generated by the instructions

```
pcb = ppcb[1];
AddCb(pcb, 1, 1, COMPLEX(2.), pcot_vtv, "t_vtv");
AddCb(pcb, 2, 1, COMPLEX(1.), pcot_vtv, "t_vtv");
```
(7.15)

The result of these assignments is shown in the test output as

```
B^2_nu1_nu2
----------------------------------
 nu1  nu2          Re B          Im B C^(1)          C^(2)          T
                                      -------------- -------------- --------------
   1    1             2             0 C_f            C_t            t_vtv
   2    1             1             0 L_f            C_t            t_vtv
```
(7.16)

Construction of a set of matrix blocks. The final stage of assembling a set of nnu matrix blocks ppcsa (Fig. 3) is carried out by the routine

```
// Allocates and computes set of near-field matrices ppcsa
// for a set of coupling coefficients B = ppcb,
// and mapping coefficients ppca1 and ppca2
// input:
// ak0          = wave number
// pcgeo1       = geometry 1
// pcgeo2       = geometry 2
// nnu          = number of matrices to be created
// ppcb         = array of nnu coupling coefficients B
// nnca1        = number of sets of mapping coefficients C^1
// nnca2        = number of sets of mapping coefficients C^2
// ppca1        = array of nnca1 sets of coefficients C^1
// ppca2        = array of nnca2 sets of coefficients C^2
// output:
// ppcsa        = array of nnu matrix blocks
void SetAAnCC(FLOAT_T ak0, CGEO *pcgeo1, CGEO *pcgeo2,
              int nnu, CBFA **ppcb,
              int nnca1, int nnca2, CCFA **ppca1, CCFA **ppca2,
              MC_CSR ***pppcsa)
```

(7.17)

in vmax_ccfa.cpp.

The routine uses as input:

1. The wave number ak0.
2. The geometries G1 and G2 (pcgeo1 and pcgeo2), set of nnu coupling-coefficient data ppcb.
3. Numbers nnca1 and nnca2 of sets of mapping coefficients $C^{(1)}$ and $C^{(2)}$ to be used in the construction (they are only used to check index values).
4. Arrays ppca1 and ppca2 of mapping coefficient data $C^{(1)}$ and $C^{(2)}$.

The output generated by the routine – a set of nnu matrices – is stored in the array of matrices ppcsa.

The general structure of the routine is summarized in the pseudo-code

```
// loops through g-element types for geometries G1 and G2
for kgt1 = 1, ... , 3
    nng1 = nngk1[kgt1] // number of g-elements of type kgt1
    // get pointer to the required type kgt1 of g-elements for geom. G1:
    pg1 = pcgeo1-> ···
    for kgt2 = 1, ... , 3
        nng1 = nngk1[kgt1] // number of g-elements of type kgt1
        // get pointer to the required type kgt2 of g-elements for geom. G2:
        pg2 = pcgeo2-> ···
        // loops through g-elements in geometries G1 and G2
        for ng1 = 1, ... , nng1
            for ng2 = 1, ... , nng2
                // compute set of basic matrix elements, store in paan
                SetAg1g2(pg1, ng1, pg2, ng2, paan)
                // loop through numbers nu of blocks to be generated
                for nu = 1, ... , nnu
                    pcb = ppcb[nu] // coupling coefficient data for the matrix block nu
                    pcob = pcb->pcob // array of coupling coefficients for sets of basis functions
                    kkcc = pcob->na // number of pairs of mapping data sets
                    ppcot = pcb->ppcot // set of tensor-component multiplication tables
                    // loop through pairs of mapping data sets (C^(1), C^(2))
                    for kcc = 1, ... , kkcc
                        // get coupling coefficient B and tensor multiplication table
                        // (for later use)
                        cb = pcob->paa[kcc] // coupling value
                        pcot = ppcot[kcc] // tensor multiplication table
                        nnat = naICOO(pcot) // number of its elements
                        // get numbers of mapping data sets (C^(1), C^(2)) (row and col.)
                        nca1 = pcob->pia[kcc]
                        nca2 = pcob->pja[kcc]
                        pca1 = ppca1[nca1] // mapping data 1
                        pca2 = ppca2[nca2] // mapping data 2
                        // get numbers of unknowns per reduced unknown
                        kkxc1 = pca1->kkx
                        kkxc2 = pca2->kkx
                        pcsr1 = pca1->pcsr // inverse mapping table 1
                        pcsr2 = pca2->pcsr // inverse mapping table 2
                        pgc1 = pca1->pgc // mapping coefficients 1
                        pgc2 = pca2->pgc // mapping coefficients 2
                        // get bounds for loops through inverse mappings elements
                        nnar11 = pcsr1->pia[ng1]
                        nnar12 = pcsr1->pia[ng1 + 1]
                        nnar21 = pcsr2->pia[ng2]
                        nnar22 = pcsr2->pia[ng2 + 1]
```

```
                        // loop through elements of of the inverse map 1
                        for nar1 = nnar11, ... , nnar12
                            nr1 = pcsr1->pja[nar1] // reduced unkn. 1 number
                            nag1 = pcsr1->paa[nar1] // dir. map. storage number 1
                            // loop through elements of of the inverse map 2
                            for nar2 = nnar21, ... , nnar22
                                nr2 = pcsr2->pja[nar2] // reduced unkn. 2 number
                                nag2 = pcsr2->paa[nar2] // dir. map. storage number 2
                                // loop through elements of the tensor multipl. table
                                for nat = 1, ... , nnat
                                    // get tensor indices
                                    ni1 = pcot->pia[nat]
                                    ni2 = pcot->pja[nat]
                                    // get basic matrix element tensor index
                                    nia = pcot->paa[nat]
                                    // get unknown numbers
                                    nx1 = kkxc1 * nr1 + ni1
                                    nx2 = kkxc2 * nr2 + ni2                              (7.18)
                                    // get mapping coefficients
                                    ac1 = pgc1[kkxc1 * nag1 + ni1]
                                    ac2 = pgc2[kkxc2 * nag2 + ni2]
                                    // multiply basic matrix element by coefficients
                                    cba = cb * ac1 * ac2 * paan[nia]
                                    // add to element in output block nu
                                    StoreAddCSRna(ppcsa[nu], nx1, nx2, cba)
                                endfor nat
                            endfor nar2
                        endfor nar1
                    endfor kcc
                endfor nu
            endfor ng2
        endfor ng1
    endfor kgt2
endfor kgt1
```

8 Summary of the developments in formulation and implementation of integral equations for elasticity

We have described the formulation of several types of integral equations we are implementing in our solver, and the detailed expressions for the resulting matrix equations. As the presented material shows, the structure of the equations is quite complex and requires a significant amount of analytic and programming work.

In the area of code implementation, we have designed a general and flexible solution scheme involving construction of the stiffness matrix, its compression, and matrix-vector multiplication routines, which allows relatively easy implementation of various types of integral equations, including volumetric and surface equations, equations based on first- and second-order formulations, and equations specially adapted to high-contrast problems, hence involving different unknown fields and treating material properties in various ways. Our general goal, however, is not to unnecessarily restrict the allowable types of equations, but rather keep the scheme open-ended and allow incorporating new formulations in a possibly straightforward way. To this end, we are developing a comprehensible and extensible library of routines for constructing particular blocks and sets of matrix elements, as well as their compressed representations, appearing in various integral-equation formulations. These routines create input data used by a general routine whose task is to assemble the entire matrix and store it in a compressed form; the overall scheme of the matrix construction is visualized in Fig. 3 and exemplified with a set of routines described in Sec. 7.3.

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